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The temperature dependence of the electron mobility in semiconductor quantum wires: fluctuation effects

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Abstract. Electron transport in semiconductor quantum wires with parabolic confined potentials is considered. Non-Markovian Langevin-like equations are derived. A correspondence between the equations obtained and the balance equations for the non-equilibrium steady state is recognized. It is shown that at high temperature the electron mobility remains almost unchanged with increasing temperature. This is due to thermal fluctuations which affect the energy-loss rate via electron–phonon scattering.

1. Introduction

Electron transport in one-dimensional (1D) and quasi-one-dimensional (Q1D) semiconductor structures has attracted considerable attention over recent years. Early motivation was provided by the suggestion that at low temperatures, when the Fermi surface is sharply defined, the elastic impurity scattering will be drastically reduced [1]. In practice, there are many features inhibiting the experimental verification of this prediction. For example, the interface quality and the influence of contacts should be mentioned. Also, at low temperatures a Luttinger liquid [2, 3] forms, which can change the transport characteristics. However, quantum wires with very high electron mobility can be fabricated on the basis of extremely pure GaAs/AlGaAs heterojunctions, where the effect of impurity on the electron transport is strongly suppressed.

In the present work we study the dissipative electron transport in quantum wires by means of microscopic theory proposed in [4–6]. We choose polar optical phonons as a dissipative environment, because the interaction with these phonons is the basic mechanism of scattering in the polar semiconductors from which quantum wires are usually produced. The confined potential is assumed to be parabolic, which is very attractive from the theoretical viewpoint, since it allows many properties to be calculated in a rigorous and analytical fashion [7–10]. For instance, carriers confined in a parabolic potential with width W and height Δ_1 only absorb light at the bare harmonic oscillator frequency defined as $\omega_0 = (8\Delta_1/mW^2)^{1/2}$, where m is the effective electron mass [7]. Such potentials can be realized experimentally by means of molecular-beam epitaxy [11, 12]. The presence of a confined potential is neglected as far as the phonons are concerned. Recent calculations of electron–optical phonon interactions based on a microscopic description of the phonons show that the assumption of unmodified bulk phonon modes provides reasonable results for the total scattering rates in GaAs/AlAs quantum wells and wires [13].

We obtain non-Markovian Langevin-like equations by means of which a unified analysis of the kinetics and fluctuations in the systems of interest is possible. These equations provide

the way for wide-ranging investigations of the electron transport and noise in quantum wires. We show that in the steady state the equations obtained describe the balances of the force and energy as well as is usually achieved on the basis of the Boltzmann equations [14] or the Lei–Ting approach [15, 16]. In the present work we concentrate on the temperature dependence of the linear electron mobility. This dependence was analysed in [16] in a very sophisticated fashion. It was shown that at high lattice temperatures the electron mobility is lower than in bulk materials. The advantage of our approach in comparison to that of Lei and Ting is the taking into account of the fluctuation effects. These effects are very important for 1D systems. For example, if they are included the polarizability becomes free of divergence and convenient for calculations [17]. In our case we show that fluctuations modify the matrix element of the electron–phonon interaction, which changes the temperature dependence of the electron mobility drastically.

As may be expected, in the initial interval, increasing of the lattice temperature is accompanied by decreasing of the electron mobility, because the number of phonons in each mode interacting with electrons, and, therefore, the energy-loss rate via electron–phonon scattering increase. However, the space scale connected with thermal fluctuations in the transverse degree of freedom increases as well. This leads to the suppression of the interaction with the phonon modes with small lengths (or large wave vectors) after ensemble averaging. These two effects compete, which gives rise to a horizontal region in the temperature dependence of the electron mobility at high temperature. We find the temperature dependences at different frequencies of the confined potential, and also show that the electron mobility is higher at smaller frequencies, in agreement with the results of [16].

2. Equations

Let the Hamiltonian of the system under study be written in the form

$$H = H_0 + H_T + H_{int} \quad (1)$$

where

$$H_0 = \frac{\mathbf{p}^2}{2m} + \frac{m\omega_0^2(x^2 + y^2)}{2} - eEz \quad (2)$$

is the Hamiltonian of an electron driven by the electric field along the z -axis and confined by the parabolic potential in the lateral plane. H_T is the thermal bath Hamiltonian and H_{int} describes the interaction of an electron with the dissipative environment. For the case of polar optical phonons this term has the form

$$\begin{aligned} H_{int}(\mathbf{r}, t) &= -L^{-3/2} \sum_k Q_k(t) \exp\{i\mathbf{k} \cdot \mathbf{r}(t)\} \\ &= e \left(\frac{2\pi\hbar\Omega_0}{L^3\kappa^*} \right)^{1/2} \sum_k \frac{i}{k} (b_k(t)e^{i\mathbf{k}\cdot\mathbf{r}(t)} - b_{-k}^+(t)e^{-i\mathbf{k}\cdot\mathbf{r}(t)}) \end{aligned} \quad (3)$$

where $1/\kappa^* = 1/\kappa_\infty - 1/\kappa_0$, where κ_∞ and κ_0 are the hf and static permittivities of a crystal, respectively, and L^3 is its volume, $\hbar\Omega_0$ is an optical phonon energy, and $b_k^+(t)$ and b_k are the creation and annihilation operators for phonons.

According to the microscopic theory proposed in [4–6], we can obtain the following non-Markovian Langevin-like equations:

$$\ddot{z}(t) - \frac{1}{mL^3} \sum_k ik_z \int dt_1 \left(M_k(t, t_1) \frac{i}{\hbar} [e^{i\mathbf{k}\cdot\mathbf{r}(t)}, e^{-i\mathbf{k}\cdot\mathbf{r}(t_1)}]_- \right)$$

$$+ \varphi_k(t, t_1) \frac{1}{2} [e^{ik \cdot r(t)}, e^{-ik \cdot r(t_1)}]_+ \Big) = \frac{e}{m} E + \xi_z(t) \quad (4)$$

$$\ddot{r}_\perp(t) + \omega_0^2 r_\perp(t) - \frac{1}{mL^3} \sum_k ik_\perp \cos \alpha \int dt_1 \left(M_k(t, t_1) \frac{i}{\hbar} [e^{ik \cdot r(t)}, e^{-ik \cdot r(t_1)}]_- \right. \\ \left. + \varphi_k(t, t_1) \frac{1}{2} [e^{ik \cdot r(t)}, e^{-ik \cdot r(t_1)}]_+ \right) = \xi_\perp(t) \quad (5)$$

where $r_\perp^2 = r_x^2 + r_y^2$, $k_\perp^2 = k_x^2 + k_y^2$, α is the angle between r_\perp and k_\perp , $[\dots]_-$ and $[\dots]_+$ indicate a commutator and an anticommutator, respectively, and $\langle \dots \rangle$ indicates a thermal averaging. $\varphi_k(t, t_1)$ and $M_k(t, t_1)$ are a linear response function and a correlation function of the unperturbed thermal bath variables, respectively. For the case of polar optical phonons we find [6]

$$\varphi_k(\tau) = \frac{4\pi\Omega_0 e^2}{k^2 \kappa^*} \sin(\Omega_0 \tau) \eta(\tau) \quad (6)$$

$$M_k(\tau) = \frac{2\pi\hbar\Omega_0 e^2}{k^2 \kappa^*} \cos(\Omega_0 \tau) \coth \frac{\hbar\Omega_0}{2T}. \quad (7)$$

Here T is the lattice temperature and $\eta(\tau)$ is a unit step function.

Fluctuation sources obtained from microscopic considerations have exact forms [4], which makes the calculation of correlation functions of any order possible. For example, the second correlator of ξ_z has the following form for the case of weak electron–environment coupling [6]:

$$\left\langle \frac{1}{2} [\xi_z(t), \xi_z(t_1)]_+ \right\rangle = \frac{1}{m^2 L^3} \sum_k \frac{k_z^2}{2} (M_k(t, t_1) \langle [e^{ik \cdot r(t)}, e^{-ik \cdot r(t_1)}]_+ \rangle \\ + R_k(t, t_1) \langle [e^{ik \cdot r(t)}, e^{-ik \cdot r(t_1)}]_- \rangle). \quad (8)$$

Here

$$R_k(\tau) = \frac{2\pi\hbar\Omega_0 e^2}{ik^2 \kappa^*} \sin(\Omega_0 \tau). \quad (9)$$

In deriving equations (4), (5), and (8) we have taken into account the influence of an electron on the heat bath, and the fact that the statistics of the unperturbed heat bath variables is Gaussian [4]. The latter assumption is valid if we neglect phonon anharmonicity.

Our prime interest here is in the electron transport along the z -axis. Separating in equation (4) the mean (\bar{z}) and fluctuation (\tilde{z}) parts, we obtain

$$m\ddot{\bar{z}}(t) = eE - G(\dot{\bar{z}}) \quad (10)$$

$$\ddot{\tilde{z}}(t) + \int dt_1 \gamma(t-t_1) \dot{\tilde{z}}(t_1) = \xi_z(t). \quad (11)$$

Equation (10) presents Newton's second law, where $G(\dot{\bar{z}})$ is a friction force. Equation (11) is the generalized non-Markovian Langevin equation. Going to a Fourier transform, we find the expression for the velocity fluctuation spectrum:

$$\left\langle \frac{1}{2} [\tilde{V}_z(\omega), \tilde{V}_z(0)]_+ \right\rangle = \frac{K_z(\omega)}{\omega^2 + \gamma^2(\omega)} \quad (12)$$

where $K_z(\omega)$ is the spectral density of fluctuation sources:

$$K_z(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \left\langle \frac{1}{2} [\xi_z(0), \xi_z(\tau)]_+ \right\rangle. \quad (13)$$

It should be noticed that both the fluctuation source and the damping coefficient in the Langevin equation, as well as the friction force, are obtained from the microscopic considerations of the electron–phonon interaction. The concrete forms of these values will be found in the next section for the non-equilibrium steady state.

3. Steady-state transport

In this section we consider the non-equilibrium steady state when the electron has a fixed drift velocity V_d and a fixed level of velocity fluctuations $V_T^2 = \langle \tilde{V}_z^2 \rangle$ along the z -axis (or a fixed electron temperature $T_e = mV_T^2$) due to the thermalization process. The drift velocity can be found from equation (10) rewritten for the steady state as

$$G(V_d) = eE \quad (14)$$

where the friction force $G(V_d)$ is

$$\begin{aligned} G(V_d) = & \frac{1}{2\sqrt{2\pi}V_T} \frac{e^2\Omega_0}{\kappa^*} \int_0^{k_D} k_\perp dk_\perp \int_0^{k_D} dk_z \frac{1}{k^2} e^{-k_\perp^2 R^2} \sum_{l=0}^{\infty} I_l \left\{ \frac{\omega_{k_\perp}}{\omega_0} \left(\sinh \frac{\hbar\omega_0}{2T} \right)^{-1} \right\} \\ & \times \left(\left(\coth \frac{\hbar\Omega_0}{2T} + 1 \right) \left(\exp \left\{ \frac{\hbar\omega_0}{2T} l \right\} \right) \left(\exp \left\{ -\frac{(\omega_{k_z} - k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \\ & - \exp \left\{ -\frac{(\omega_{k_z} + k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \\ & + \exp \left\{ -\frac{\hbar\omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{k_z} - k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \\ & - \exp \left\{ -\frac{(\omega_{k_z} + k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \left. \right) \\ & + \left(\left(\coth \frac{\hbar\Omega_0}{2T} - 1 \right) \left(\exp \left\{ \frac{\hbar\omega_0}{2T} l \right\} \right) \left(\exp \left\{ -\frac{(\omega_{k_z} - k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \\ & - \exp \left\{ -\frac{(\omega_{k_z} + k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \\ & + \exp \left\{ -\frac{\hbar\omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{k_z} - k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \\ & - \exp \left\{ -\frac{(\omega_{k_z} + k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \left. \right) \left. \right). \end{aligned} \quad (15)$$

Here $\omega_{k_\perp} = \hbar k_\perp^2/2m$, $\omega_{k_z} = \hbar k_z^2/2m$, $R^2 = (\hbar/2m\omega_0) \coth(\hbar\omega_0/2T)$, and $\tau = t - t_1$, and the $I_l(x)$ are the modified Bessel functions. The calculation of this expression is presented in the appendix.

For the case of weak electron–phonon coupling, the dispersion of the electron velocity fluctuations is obtained as follows [6]:

$$V_T^2 = \frac{K_z(0)}{2\gamma(0)} \quad (16)$$

where the expressions for $K_z(0)$ and $\gamma_z(0)$ are presented in the appendix as well.

To gain a better understanding and to compare with standard approaches, we rewrite equation (16) as an energy balance equation:

$$P_E = P_{ph} + P_{osc} \quad (17)$$

where

$$P_E = eEV_d = G(V_d)V_d \quad (18)$$

is an energy supplied by the external force,

$$\begin{aligned} P_{ph} = \hbar\Omega_0 \sum_k \frac{dN_k}{dt} = \hbar\Omega_0 \sum_k \frac{2\pi}{\hbar} \frac{2\pi e^2 \hbar \Omega_0}{\kappa^* k^2} \frac{1}{\sqrt{2\pi} \hbar k_z V_T} \exp\{-k_{\perp}^2 R^2\} \\ \times \sum_{l=0}^{\infty} I_l \left\{ \frac{\omega_{k\perp}}{\omega_0} \left(\sinh \frac{\hbar\omega_0}{2T} \right)^{-1} \right\} \left((N_0 + 1) \left(\exp \left\{ \frac{\hbar\omega_0}{2T} l \right\} \right. \right. \\ \times \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \\ \left. \left. + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right. \\ \left. \left. + \exp \left\{ -\frac{\hbar\omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \right. \\ \left. \left. \left. + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right) \right) \\ - N_0 \left(\exp \left\{ \frac{\hbar\omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \\ \left. \left. + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right. \\ \left. \left. + \exp \left\{ -\frac{\hbar\omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \right. \\ \left. \left. \left. + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right) \right) \right) \right) \quad (19) \end{aligned}$$

is an energy loss rate via electron-phonon scattering, and

$$\begin{aligned} P_{osc} = \sum_k \frac{2\pi}{\hbar} \frac{2\pi e^2 \hbar \Omega_0}{\kappa^* k^2} \frac{1}{\sqrt{2\pi} \hbar k_z V_T} \exp\{-k_{\perp}^2 R^2\} \\ \times \sum_{l=0}^{\infty} (\hbar l \omega_0) I_l \left\{ \frac{\omega_{k\perp}}{\omega_0} \left(\sinh \frac{\hbar\omega_0}{2T} \right)^{-1} \right\} \left((N_0 + 1) \left(\exp \left\{ \frac{\hbar\omega_0}{2T} l \right\} \right. \right. \\ \times \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \\ \left. \left. + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right. \\ \left. \left. - \exp \left\{ -\frac{\hbar\omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \right. \\ \left. \left. \left. + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right) \right) \\ \left. \left. + N_0 \left(\exp \left\{ \frac{\hbar\omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \right. \right. \right) \end{aligned}$$

$$\begin{aligned}
& + \exp\left\{-\frac{(\omega_{kz} + k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2}\right\} \\
& - \exp\left\{-\frac{\hbar\omega_0}{2T}l\right\} \left(\exp\left\{-\frac{(\omega_{kz} - k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2}\right\}\right. \\
& \left. + \exp\left\{-\frac{(\omega_{kz} + k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2}\right\}\right) \quad (20)
\end{aligned}$$

is an energy transferred to the transverse degrees of freedom. Here

$$N_0 = (\exp\{\hbar\Omega_0/T\} - 1)^{-1}$$

is an equilibrium phonon distribution function.

As may be seen from these expressions, if we neglect fluctuations $V_T^2 \rightarrow 0$, then

$$\frac{1}{\sqrt{2\pi\hbar k_z V_T}} \exp\left\{-\frac{(\omega_{kz} \pm k_z V_d \pm \Omega_0 \pm l\omega_0)^2}{2k_z^2 V_T^2}\right\} \rightarrow \delta(\hbar\omega_{kz} \pm \hbar k_z V_d \pm \hbar\Omega_0 \pm \hbar l\omega_0)$$

i.e. the electron–phonon interaction is described by the well-known Fermi ‘golden rule’ with the modified matrix element

$$|S(k)|^2 = \frac{2\pi e^2 \hbar \Omega_0}{\kappa^* k^2} \exp\left\{-\frac{\hbar k_{\perp}^2}{2m\omega_0} \coth\left(\frac{\hbar\omega_0}{2T}\right)\right\} I_l \left\{ \frac{\omega_{k\perp}}{\omega_0} \left(\sinh \frac{\hbar\omega_0}{2T}\right)^{-1} \right\}. \quad (21)$$

Of special interest is the factor

$$\exp\left\{-\frac{\hbar k_{\perp}^2}{2m\omega_0} \coth\left(\frac{\hbar\omega_0}{2T}\right)\right\}$$

in the modified matrix element. It arises even if $l = 0$, i.e. if the phonon emission (absorption) is not attended by transfers between the oscillator levels. This factor is due to ensemble averaging, which suppresses the interaction with phonon modes with large transverse wave vectors, i.e. with wavelengths much less than the root mean square of the transverse coordinate fluctuations.

The balance equations derived look like that obtained from the Boltzmann equations [14] or from the Lei–Ting approach [15]. However, if thermal fluctuations are taken into consideration, this affects the transport characteristics of quantum wires significantly. Longitudinal fluctuations smear out δ -functions while transverse fluctuations modify the matrix element of the electron–phonon interaction.

It is interesting to note that in the above expressions the terms corresponding to the excitation of the transverse degrees of freedom are multiplied by the factor $\exp\{\hbar l\omega_0/2T\}$ and the terms corresponding to the damping of the transverse degrees of freedom are multiplied by the factor $\exp\{-\hbar l\omega_0/2T\}$. The condition $V_T^2 = T/m$ is fulfilled for the equilibrium case ($V_d = 0$) due to these factors.

4. Results and discussion

In the previous section we have derived equations describing steady-state transport in semiconductor quantum wires with parabolic confined potentials. The detailed analysis of these equations will be very interesting, but in the present work we concentrate on the study of the temperature dependence of the electron mobility. The weak-field regime is considered, so that the linear mobility $\mu = V_d/E$ describes the electron transport completely. Solving equations (14) and (16) self-consistently, we have found μ as a function of the lattice temperature T . This dependence is presented in figure 1 for the drift velocity $V_d = 0.01 V_0$,

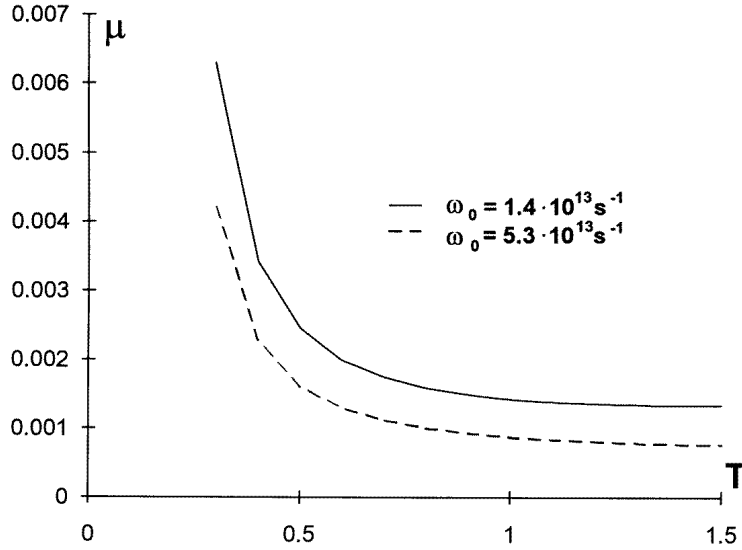


Figure 1. The temperature dependences of the linear electron mobility at different frequencies of the confined potential. The temperature is normalized to $T_0 = 408$ K, and the electron mobility is normalized to $\mu_0 = 836 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$.

where $V_0 = (\hbar\Omega_0/2m)^{1/2}$. The temperature is normalized to $T_0 = \hbar\Omega_0/k_B$, and the electron mobility is normalized to $\mu_0 = V_0/E_0$, where $eE_0 = \lambda(m\hbar\Omega_0^3/\pi)^{1/2}$, and

$$\lambda = \frac{e^2}{2\kappa^*\hbar\Omega_0} \left(\frac{2m\Omega_0}{\hbar} \right)^{1/2}$$

is the constant of the electron–phonon interaction. If the quantum wire under study is fabricated on the basis of a GaAs/AlAs heterojunction, then $m = 0.067m_e$, $T_0 = 408$ K, $1/\kappa^* = 0.0069$, $\lambda = 0.069 \ll 1$, $E_0 = 6560 \text{ V cm}^{-1}$, $V_0 = 2.2 \times 10^7 \text{ cm s}^{-1}$, and $\mu_0 = 836 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$.

The solid line represents the typical experimental situation, where the parabolic potential has the width $W = 4 \times 10^{-5} \text{ cm}$ and the height $\Delta_1 = 150 \text{ meV}$, which gives the value $\omega_0 = (8\Delta_1/mW^2)^{1/2} = 1.4 \times 10^{13} \text{ s}^{-1}$.

One can see that increasing of the temperature is accompanied by decreasing of the linear mobility over the initial interval, and that subsequently the curve flattens out. This horizontal region is caused by the competition of two effects. Increasing of the temperature leads to increasing of the phonon number in each mode interacting with the electron, and meanwhile leads to increasing of the variance of the transverse coordinate fluctuations $R^2 = (\hbar/2m\omega_0) \coth(\hbar\omega_0/2T)$. These fluctuations suppress the interaction with the phonon modes with small wavelengths as a result of ensemble averaging. The first effect increases the energy-loss rate via electron–phonon scattering, while the second one decreases this rate.

To compare our results with those of Wang and Lei [16], we also present the temperature dependence of the electron mobility for another frequency of the confined potential (the dashed line). As may be seen, the smaller the confined frequency, the larger the electron mobility, which is in agreement with the conclusions of [16].

In closing, it cannot be too highly stressed that fluctuation effects are of fundamental

importance in the physics of semiconductor nanostructures. It may be safely asserted that a better understanding will be gained if they are taken into consideration.

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Appendix. Calculation of the expressions for the friction force, the damping coefficient, and the spectral density of the fluctuation sources

To calculate these expressions, we assume that the non-Markovian equations (4) and (5) have a some scale of time non-locality τ_c and neglect the relaxation and the influence of fluctuation sources in the time period around τ_c . In this case the time evolution of the coordinate operators is described by the following expressions:

$$z(t) = z(t_1) + V_z(t_1)(t - t_1) \quad (\text{A1})$$

$$r_{\perp}(t) = r_{\perp}(t_1) \cos \omega_0(t - t_1) + \frac{V_{\perp}(t_1)}{\omega_0} \sin \omega_0(t - t_1). \quad (\text{A2})$$

We use the Baker–Hausdorff formula

$$e^{-i\mathbf{k}\cdot\mathbf{r}(t)} e^{i\mathbf{k}\cdot\mathbf{r}(t_1)} = \exp\{i\mathbf{k}\cdot(\mathbf{r}(t) - \mathbf{r}(t_1))\} \exp\left\{\frac{k^2}{2}[\mathbf{r}(t_1), \mathbf{r}(t)]_{-}\right\}$$

and the following formulae for the commutators ($[A, b]_{-} = [B, a]_{-} = 0$):

$$[AB, ab]_{-} = \frac{1}{2}([A, a]_{-}[B, b]_{+} + [A, a]_{+}[B, b]_{-})$$

$$[AB, ab]_{+} = \frac{1}{2}([A, a]_{+}[B, b]_{+} + [A, a]_{-}[B, b]_{-}).$$

As a result we obtain the expressions for the commutator and anticommutator:

$$\begin{aligned} [\exp\{i\mathbf{k}\cdot\mathbf{r}(t)\}, \exp\{-i\mathbf{k}\cdot\mathbf{r}(t_1)\}]_{+} &= \left(\cos\left(\frac{\hbar k_z^2}{2m}\tau\right) \cos\left(\frac{\hbar k_{\perp}^2}{2m\omega_0} \sin \omega_0\tau\right) \right. \\ &\quad \left. - \sin\left(\frac{\hbar k_z^2}{2m}\tau\right) \sin\left(\frac{\hbar k_{\perp}^2}{2m\omega_0} \sin \omega_0\tau\right) \right) \Lambda_{\perp}(t, t_1) \Lambda_z(t, t_1) \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} [\exp\{i\mathbf{k}\cdot\mathbf{r}(t)\}, \exp\{-i\mathbf{k}\cdot\mathbf{r}(t_1)\}]_{-} &= \frac{2}{i} \left(\cos\left(\frac{\hbar k_z^2}{2m}\tau\right) \sin\left(\frac{\hbar k_{\perp}^2}{2m\omega_0} \sin \omega_0\tau\right) \right. \\ &\quad \left. + \sin\left(\frac{\hbar k_z^2}{2m}\tau\right) \cos\left(\frac{\hbar k_{\perp}^2}{2m\omega_0} \sin \omega_0\tau\right) \right) \Lambda_{\perp}(t, t_1) \Lambda_z(t, t_1). \end{aligned} \quad (\text{A4})$$

Here $\tau = t - t_1$,

$$\Lambda_{\perp}(t, t_1) = \exp\{i\mathbf{k}_{\perp}\cdot(\mathbf{r}_{\perp}(t) - \mathbf{r}_{\perp}(t_1))\}$$

$$\Lambda_z(t, t_1) = \exp\{ik_z(z(t) - z(t_1))\}.$$

We separate the functions $\Lambda_{\perp}(t, t_1)$ and $\Lambda_z(t, t_1)$ into mean and fluctuation parts:

$$\Lambda_{\perp}(t, t_1) = \bar{\Lambda}_{\perp}(t, t_1) + \tilde{\Lambda}_{\perp}(t, t_1)$$

$$\Lambda_z(t, t_1) = \bar{\Lambda}_z(t, t_1) + \tilde{\Lambda}_z(t, t_1).$$

The function $\bar{\Lambda}_z(t, t_1)$ may be written as

$$\bar{\Lambda}_z(t, t_1) = \exp\{ik_z V_d \tau\} \Theta_{V_z}(k_z, \tau)$$

where

$$\Theta_{V_z}(k_z, \tau) = \langle \exp\{ik_z \tilde{V}_z \tau\} \rangle$$

is a generating function for velocity fluctuations along the z -axis. If the velocity fluctuations are Gaussian, this function has the form

$$\Theta_{V_z}(k_z, \tau) = \exp\left\{-\frac{k_z^2}{2} V_T^2 \tau^2\right\}. \quad (\text{A5})$$

Thus

$$\bar{\Lambda}_z(t, t_1) = \exp\{ik_z V_d \tau\} \exp\left\{-\frac{k_z^2}{2} V_T^2 \tau^2\right\} \quad (\text{A6})$$

$$\tilde{\Lambda}_z(t, t_1) = ik_z(z(t) - z(t_1)) \bar{\Lambda}_z(t, t_1). \quad (\text{A7})$$

The validity of the Gaussian approximation was discussed in [6]. At least for the case of a weak electric field when the current–voltage characteristic is ohmic we can assume the velocity fluctuation to be Gaussian without serious consequences. It is evident that

$$\tau_c = \frac{\sqrt{2}}{k_z V_T}.$$

Let us next consider the motion in the lateral plane. We separate $\mathbf{r}_\perp(t)$ into mean ($\bar{\mathbf{r}}_\perp(t)$) and fluctuation ($\tilde{\mathbf{r}}_\perp(t)$) parts. The amplitude of the oscillation will be considered to be small, and we can expand the function $\exp\{i\mathbf{k}_\perp \cdot (\tilde{\mathbf{r}}_\perp(t) - \tilde{\mathbf{r}}_\perp(t_1))\}$:

$$\exp\{i\mathbf{k}_\perp \cdot (\tilde{\mathbf{r}}_\perp(t) - \tilde{\mathbf{r}}_\perp(t_1))\} = 1 + i\mathbf{k}_\perp \cdot \left((1 - \cos \omega_0 \tau) \bar{\mathbf{r}}_\perp + \frac{\sin \omega_0 \tau}{\omega_0} \tilde{\mathbf{V}}_\perp \right)$$

In the case of Gaussian fluctuations we can write

$$\langle \exp\{i\mathbf{k}_\perp \cdot (\tilde{\mathbf{r}}_\perp(t) - \tilde{\mathbf{r}}_\perp(t_1))\} \rangle = \exp\left\{-\frac{k_\perp^2}{2} (\langle \tilde{r}_\perp^2(t) \rangle + \langle \tilde{r}_\perp^2(t_1) \rangle - \langle [\tilde{r}_\perp(t), \tilde{r}_\perp(t_1)]_+ \rangle)\right\}. \quad (\text{A8})$$

The non-equilibrium state in the lateral plane is induced by the non-linearity of the electron–environment interaction. Because of this, in the case of weak coupling and a weak field the transverse motion in the time period around τ_c may be considered to be equilibrium motion. Therefore, we can find the correlator of the coordinate fluctuations by means of the linear fluctuation-dissipation theorem:

$$\left\langle \frac{1}{2} [\tilde{r}_\perp(t), \tilde{r}_\perp(t_1)]_+ \right\rangle = R^2 \cos \omega_0 \tau \quad (\text{A9})$$

where

$$R^2 = \frac{\hbar}{2m\omega_0} \coth\left(\frac{\hbar\omega_0}{2T}\right).$$

Here T is a temperature of the thermal bath. Finally we obtain

$$\bar{\Lambda}_\perp(t, t_1) = \left(1 + i\mathbf{k}_\perp \cos \alpha \left((1 - \cos \omega_0 \tau) \bar{\mathbf{r}}_\perp + \frac{\sin \omega_0 \tau}{\omega_0} \tilde{\mathbf{V}}_\perp \right) \right) \exp\{-k_\perp^2 R^2 (1 - \cos \omega_0 \tau)\}. \quad (\text{A10})$$

To ease the calculation, we rewrite the equations as follows:

$$\begin{aligned} & \cos\left(\frac{\hbar k_{\perp}^2}{2m\omega_0} \sin \omega_0 \tau\right) \exp\left\{\frac{\hbar k_{\perp}^2}{2m\omega_0} \cos \omega_0 \tau \coth \frac{\hbar \omega_0}{2T}\right\} \\ &= I_0 \left\{ \frac{\hbar k_{\perp}^2}{2m\omega_0} \left(\sinh \frac{\hbar \omega_0}{2T} \right)^{-1} \right\} + 2 \sum_{l=1}^{\infty} I_l \left\{ \frac{\hbar k_{\perp}^2}{2m\omega_0} \left(\sinh \frac{\hbar \omega_0}{2T} \right)^{-1} \right\} \\ & \quad \times \cos(l\omega_0 \tau) \cosh\left(\frac{\hbar \omega_0}{2T} l\right) \end{aligned} \quad (\text{A11})$$

$$\begin{aligned} & \sin\left(\frac{\hbar k_{\perp}^2}{2m\omega_0} \sin \omega_0 \tau\right) \exp\left\{\frac{\hbar k_{\perp}^2}{2m\omega_0} \cos \omega_0 \tau \coth \frac{\hbar \omega_0}{2T}\right\} \\ &= 2 \sum_{l=1}^{\infty} I_l \left\{ \frac{\hbar k_{\perp}^2}{2m\omega_0} \left(\sinh \frac{\hbar \omega_0}{2T} \right)^{-1} \right\} \sin(l\omega_0 \tau) \sinh\left(\frac{\hbar \omega_0}{2T} l\right) \end{aligned} \quad (\text{A12})$$

where the $I_l\{x\}$ are modified Bessel functions.

Substituting the commutators and the functions $\varphi_k(\tau)$, $M_k(\tau)$, and $R_k(\tau)$ into equations (4) and (5) and integrating with respect to τ , we finally obtain the expressions for the friction force $G(V_d)$ (15) as well as for the damping coefficient and the spectral density of fluctuation sources at zero frequency, $\gamma(0)$ and $K(0)$, respectively:

$$\begin{aligned} K_z(0) &= \frac{1}{2\sqrt{2\pi} V_T} \frac{\hbar e^2 \Omega_0}{m^2 \kappa^*} \int_0^{k_D} k_{\perp} dk_{\perp} \int_0^{k_D} k_z dk_z \frac{1}{k^2} e^{-k_{\perp}^2 R^2} \sum_{l=0}^{\infty} I_l \left\{ \frac{\omega_{k\perp}}{\omega_0} \left(\sinh \frac{\hbar \omega_0}{2T} \right)^{-1} \right\} \\ & \quad \times \left(\left(\coth \frac{\hbar \Omega_0}{2T} + 1 \right) \left(\exp \left\{ \frac{\hbar \omega_0}{2T} l \right\} \right) \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right. \\ & \quad + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \\ & \quad + \exp \left\{ -\frac{\hbar \omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \\ & \quad + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \left. \right) \\ & \quad + \left(\left(\coth \frac{\hbar \Omega_0}{2T} - 1 \right) \left(\exp \left\{ \frac{\hbar \omega_0}{2T} l \right\} \right) \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right) \right. \\ & \quad + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \\ & \quad + \exp \left\{ -\frac{\hbar \omega_0}{2T} l \right\} \left(\exp \left\{ -\frac{(\omega_{kz} - k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \\ & \quad + \exp \left\{ -\frac{(\omega_{kz} + k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2} \right\} \left. \right) \left. \right) \end{aligned} \quad (\text{A13})$$

$$\begin{aligned} \gamma_z(0) &= \frac{1}{2\sqrt{2\pi} V_T^3} \frac{e^2 \Omega_0}{m \kappa^*} \int_0^{k_D} k_{\perp} dk_{\perp} \int_0^{k_D} dk_z \frac{1}{k_z k^2} e^{-k_{\perp}^2 R^2} \sum_{l=0}^{\infty} I_l \left\{ \frac{\omega_{k\perp}}{\omega_0} \left(\sinh \frac{\hbar \omega_0}{2T} \right)^{-1} \right\} \\ & \quad \times \left(\left(\coth \frac{\hbar \Omega_0}{2T} + 1 \right) \left(\exp \left\{ \frac{\hbar \omega_0}{2T} l \right\} \right) \right. \\ & \quad \times \left((\omega_{kz} - k_z V_d + \Omega_0 + l\omega_0) \exp \left\{ -\frac{(\omega_{kz} - k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2} \right\} \right. \end{aligned}$$

$$\begin{aligned}
& + (\omega_{kz} + k_z V_d + \Omega_0 + l\omega_0) \exp\left\{-\frac{(\omega_{kz} + k_z V_d + \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2}\right\} \\
& + \exp\left\{-\frac{\hbar\omega_0}{2T}l\right\} \left((\omega_{kz} - k_z V_d + \Omega_0 - l\omega_0) \right. \\
& \times \exp\left\{-\frac{(\omega_{kz} - k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2}\right\} \\
& + (\omega_{kz} + k_z V_d + \Omega_0 - l\omega_0) \exp\left\{-\frac{(\omega_{kz} + k_z V_d + \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2}\right\} \left. \right) \\
& + \left(\left(\coth \frac{\hbar\Omega_0}{2T} - 1 \right) \left(\exp\left\{\frac{\hbar\omega_0}{2T}l\right\} \right. \right. \\
& \times \left((\omega_{kz} - k_z V_d - \Omega_0 + l\omega_0) \exp\left\{-\frac{(\omega_{kz} - k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2}\right\} \right. \\
& + (\omega_{kz} + k_z V_d - \Omega_0 + l\omega_0) \exp\left\{-\frac{(\omega_{kz} + k_z V_d - \Omega_0 + l\omega_0)^2}{2k_z^2 V_T^2}\right\} \left. \right) \\
& + \exp\left\{-\frac{\hbar\omega_0}{2T}l\right\} \left((\omega_{kz} - k_z V_d - \Omega_0 - l\omega_0) \right. \\
& \times \exp\left\{-\frac{(\omega_{kz} - k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2}\right\} \\
& + (\omega_{kz} + k_z V_d - \Omega_0 - l\omega_0) \exp\left\{-\frac{(\omega_{kz} + k_z V_d - \Omega_0 - l\omega_0)^2}{2k_z^2 V_T^2}\right\} \left. \right) \left. \right).
\end{aligned} \tag{A14}$$

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