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# Self-Consistent Approximation for Electron–Optical-Phonon Interaction in a Quantum Wire

N. Mori, H. Momose, and C. Hamaguchi

*Department of Electronic Engineering, Osaka University, 2–1 Yamada-oka, Suita City, Osaka 565, Japan*
*Fax: +81-6-879-7753; e-mail: mori@ele.eng.osaka-u.ac.jp*

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A spectral density function $A(k,\omega)$ for an electron in a quantum wire interacting with longitudinal-optical-phonons is calculated in a self-consistent manner. The method gives us a natural way to handle the singularities in the density of states and the scattering rates. The obtained spectral density function exhibits a resonant polaron effect at around $\omega = \omega_0$, where $\omega_0$ is the longitudinal-optical-phonon energy. The drift velocity is then evaluated by performing the Monte Carlo simulation in $(k,\omega)$-space using the spectral density function for a GaAs quantum wire with parabolic confining potential of $\Omega = 2\omega_0$ at room temperature. The drift velocity for applied electric fields up to $F = 1\,\mathrm{kV/cm}$ is found to be significantly lower than that calculated by a Monte Carlo simulation based on the semi-classical Boltzmann transport equation.

It was theoretically pointed out that a drastic increase of electron mobility in a quantum wire is expected at low temperatures because of suppression of impurity scattering, which inevitably accompanies large momentum changes of $2k_{\mathrm{F}}$ for one-dimensional electron gases (1DEG) [1]. Electron–longitudinal-optical (LO) phonon interaction, however, plays an important role in electron transport in compound semiconductors at high temperatures, and the situation is quite different from that at low temperatures. For a system having low electron density, no sharp Fermi surface exists at high temperatures, and the transport properties at low and moderate electric fields are governed mainly by scattering rates, $W(\varepsilon)$, for electrons with low kinetic energy $\varepsilon$, which contrasts with the low temperature case where only $W(\varepsilon)$ at $\varepsilon = \varepsilon_{\mathrm{F}}$ affects the electron mobility. Since the scattering rates are proportional to the product of the final density of states, $D(\varepsilon)$, and the matrix elements, the LO phonon scattering rate for 1DEG has singularity at the onset of LO phonon emission due to the singularity of $D(\varepsilon)$ at $\varepsilon = 0$. This singularity of $W(\varepsilon)$ in turn affects $D(\varepsilon)$, and thus $W(\varepsilon)$ and $D(\varepsilon)$ should be calculated self-consistently. In the present study, we calculate a spectral density function for a one-dimensional electron interacting with LO phonons in a self-consistent manner to obtain the self-consistent scattering rates and density of states, and perform a Monte Carlo (MC) simulation to evaluate the drift velocity, which is then compared with the results obtained by a semi-classical MC simulation.

For an electron in a quantum wire interacting with LO phonons, the electron has a finite lifetime when it is scattered, and there is some uncertainty in its momentum, $k$, or energy, $\omega$, or both. We should, therefore, treat $k$ and $\omega$ as separate variables, and the spectral density function, $A(k,\omega)$, gives us the probability that the electron has momen-

tum $k$ and energy $\omega$ [2]. Once $A(k,\omega)$ is known, we can evaluate physical quantities, such as scattering rates and density of states in the present case, by summing over $k$ and/or $\omega$ with $A(k,\omega)$ of the probability weight. Since $A(k,\omega)$ is given by the imaginary part of the retarded Green's function for an electron, $G_{\rm ret}(k,\omega)$, multiplied by $-2$, and $G_{\rm ret}(k,\omega)$ can be calculated from the Matsubara Green's function, $G(k,i\omega_n)$, through an analytic continuation, we have

$$A(k,\omega) = -2\Im G(k,\omega+i0) = -2\Im\,\frac{1}{\omega+i0-\Sigma(k,\omega+i0)-\varepsilon_k}\,, \tag{1}$$

where $\Sigma(k,i\omega_n)$ is the self-energy of the electron due to the interaction with LO phonons, and $\varepsilon_k$ the *semi-classical* energy dispersion which we assume a parabolic band with effective mass $m$. Note that we use the zero field theory for evaluating $A(k,\omega)$ and therefore effects of electric field on $A(k,\omega)$, such as intracollisional field effect, are completely neglected. The diagrammatic representation of the self-consistent approximation scheme used in the present investigation is shown in Fig. 1, and the self-energy $\Sigma$ becomes

$$\Sigma(k,\omega) = \sum_{\eta=\pm1}\sum_{q}\left(N_0+\tfrac{1}{2}+\tfrac{1}{2}\,\eta\right)M_q^2\,\frac{1}{\omega-\eta\omega_0-\varepsilon_{k+q}-\Sigma(k+q,\omega-\eta\omega_0)}\,, \tag{2}$$

with $N_0$ being the LO phonon occupation number, $\omega_0$ the LO phonon energy, and $M_q$ the effective one-dimensional potential for the electron–LO phonon interaction. We solved this self-consistent equation numerically for the GaAs quantum wire with a parabolic confining potential of $\Omega = 2\omega_0$ (see [3] for the of the quantum wire), and evaluated $A(k,\omega)$ by using Eq. (1). In the present study, we neglect any effects of interfaces on phonons, and use the electron–bulk LO phonon interaction potential for $M_q$. Fig. 2 shows a contour plot of $A(k,\omega)$ for $N_0 = 0.3$, which corresponds to room temperature, together with the density of states $D(\omega) \equiv \pi^{-1}\sum_k A(k,\omega)$ in the inset. For a noninteracting electron, $A(k,\omega) = 2\pi\delta(\omega-\varepsilon_k)$ and $A(k,\omega)$ has nonzero value only on the semi-classical energy dispersion, that is shown as a dashed line in Fig. 2. As seen in the figure, the electron–LO phonon interaction makes $A(k,\omega)$ broaden. For $\omega \ll \omega_0$, the dispersion moves to lower energy by the polaronic binding energy, which is found to be $1.64\alpha\omega_0$, where $\alpha$ is the Fröhlich coupling constant. As the electron energy increases toward $\omega_0$, the polaronic effective mass becomes heavier, and a resonant polaron effect occurs at $\omega \approx \omega_0$. For $\omega\omega_0$, extrema in $A(k,\omega)$ almost follow the semi-classical energy dispersion, while the level width is quite broad, for example $\Gamma_{\rm FWHM} \approx 4\alpha\omega_0$ at $k = 1.2k_0$ while $\Gamma_{\rm FWHM} \approx \alpha\omega_0$ at $k = 0.6k_0$. The level width becomes, however, narrower for higher energy, for example $\Gamma_{\rm FWHM} \approx 2\alpha\omega_0$ at $k = 2.4k_0$, since we took only the lowest subband into account.

We treat $k$ and $\omega$ as separate variables, and it is natural to simulate an electron in $(k,\omega)$-space to study the transport properties. We adopted the MC simulation in $(k,\omega)$-

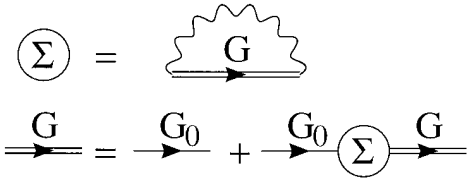


Fig. 1. Diagrammatic representation of the present approximation. The wavy line represents the interaction with LO phonons, and $G_0$ the non-interacting Green's function for an electron

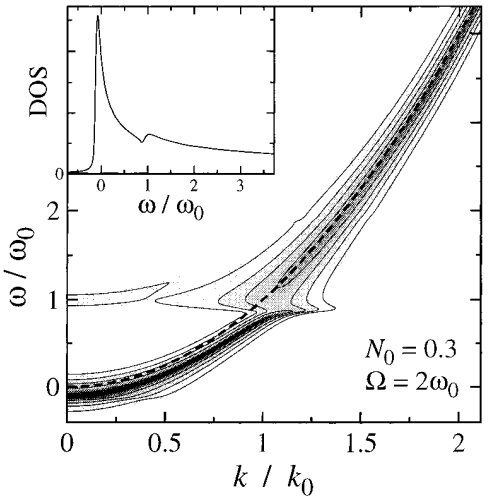


Fig. 2. A contour plot of the spectral density function, $A(k,\omega)$, for an electron in a quantum wire with a parabolic confining potential of $\Omega = 2\omega_0$ at room temperature. $\omega$ is normalized by the LO phonon energy $\omega_0$, while $k$ by $k_0 \equiv (2m\omega_0)^{1/2}$. The dashed line shows the semi-classical energy dispersion of $\omega = k^2/2m$. The density of states $D(\omega)$ is also shown in the inset

space [3] based on a quantum transport equation (QTE) [4] in the present analysis, and calculated electric field dependence of the drift velocity using the spectral density function obtained above. In order to perform the MC simulation, it it necessary to evaluate the transition probability, $S(k,\omega;k',\omega')$, per unit time from $(k,\omega)$ to $(k',\omega')$, which is given by

$$S(k,\omega;k',\omega') = 2\pi A(k',\omega') \sum_{\eta=\pm 1} \sum_{q} M_q^2 (N_0 + \tfrac{1}{2} + \tfrac{1}{2}\eta)\, \delta(\omega' + \eta\omega_0 - \omega)\, \delta_{k',k+q} \ . \tag{3}$$

The scattering rates, $W(k,\omega)$, can be calculated from $S(k,\omega;k',\omega')$ by summing over $k'$ and $\omega'$ [4]. The total scattering rate *on the mass shell*, $W(k,\varepsilon_k)$, is plotted in the inset of Fig. 3. Note that the MC simulation was done considering $S(k,\omega;k',\omega')$ and $W(k,\omega)$. For illustration only those have been represented by $W(k,\varepsilon_k)$.

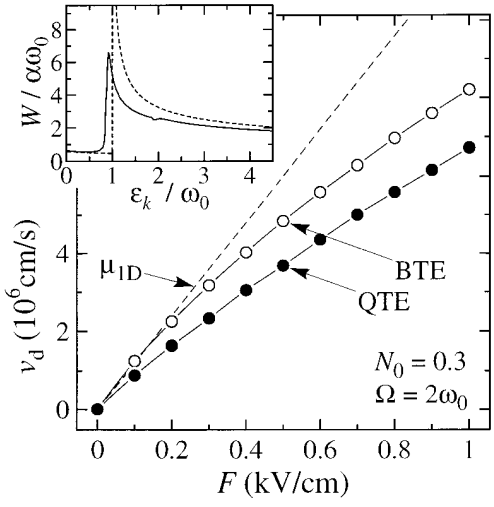


Fig. 3. Electric field dependence of drift velocity calculated by the Monte Carlo simulation based on a quantum transport equation (solid circles) and the Boltzmann transport equation (open circles). The dashed line shows the results obtained by the linear response theory. The total scattering rate *on the mass shell* is also shown as a function of $\varepsilon_k$ $(= k^2/2m)$ in the inset, together with the scattering rate for $A(k,\omega) = 2\pi\delta(\omega - \varepsilon_k)$ (dashed line in the inset)

Fig. 3 shows the calculated results of drift velocity, $v_{\mathrm{d}}$, as a function of applied electric field, $F$. We also plotted $v_{\mathrm{d}}$ calculated by using the semi-classical Boltzmann transport equation (BTE), where $A(k,\omega)$ is set to be $2\pi\,\delta(\omega-\varepsilon_k)$ since we cannot handle the broaden $A(k,\omega)$ consistently in the MC simulation based on the BTE. We find that $v_{\mathrm{d}}$ for applied electric fields up to $F=1\,\mathrm{kV/cm}$ is about 20% lower than that calculated by the MC simulation based on th BTE. This reduction in $v_{\mathrm{d}}$ may be attributed to the fact that the uncertainty in $\omega$ increase the number of scattering channels. For example, only an electron having energy greater than $\omega_0$ can emit an LO phonon for the BTE (with $A(k,\omega)=2\pi\delta(\omega-\varepsilon_k)$), while any electron has a finite probability to emit an LO phonon for the QTE (with the broadened $A(k,\omega)$), and for an electron with a fixed energy only two types of emission (or absorption) processes exist, i.e. the forward and backward scatterings, in the BTE, while any electron with a fixed energy has an infinite number of scattering channels in the QTE.

In summary, we evaluated the spectral density function for an electron in a quantum wire taking care of self-consistency between the density of states and the LO phonon scattering rates. We then performed the MC simulation in $(k,\omega)$-space, and found that $v_{\mathrm{d}}$ for applied electric fields up to $F=1\,\mathrm{kV/cm}$ is significantly lower than that calculated by a MC simulation based on the BTE.

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