Effects of impurity scattering on electron-phonon resonances in semiconductor superlattice high-field transport

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Abstract

A non-equilibrium Green’s function method is applied to model high-field quantum transport and electron-phonon resonances in semiconductor superlattices. The field-dependent density of states for elastic (impurity) scattering is found non-perturbatively in an approach which can be applied to both high and low electric fields. $I-V$ curves, and specifically electron-phonon resonances, are calculated by treating the inelastic (LO phonon) scattering perturbatively. Calculations show how strong impurity scattering suppresses the electron-phonon resonance peaks in $I-V$ curves, and their detailed sensitivity to the size, strength and concentration of impurities.
I. INTRODUCTION

There has been tremendous interest in the electron transport properties of semiconductor superlattices (SLs) since the pioneering work of Esaki and Tsu\textsuperscript{12}. Bragg scattering of carriers from the Brillouin zone boundaries of a crystal produces Bloch oscillations, or, equivalently, localized (Wannier-Stark) states within each unit cell period if the system is sufficiently clean. This regime is characterized by negative differential conductance (NDC) at sufficiently high fields, and occurs if the Bloch frequency $\Omega = eF L / \hbar$ ($F$ is the electric field and $L$ the unit cell period) is larger than the effective scattering rate $1/\tau_{\text{eff}}$. The large unit cell of the superlattice can allow electrons in a SL to perform these Bloch oscillations before being scattered\textsuperscript{13,14,15,16}. If the electric potential drop across $n$ unit cells corresponds to an optical phonon energy, Bryksin and Firsov\textsuperscript{7} predicted another high-field effect: so-called electron-phonon resonances, where an LO phonon mediates a transition between localized Wannier-Stark states whose energy separation equals the phonon energy. These resonances manifest as peaks in the current-voltage relationship and produce a nonmonotonic current-voltage dependence. Experimental $I-V$ characteristics of cubic ZnS films have been identified with such resonances\textsuperscript{8}. Growing interest in the transport properties of semiconductor superlattices, e.g. GaAs/AlAs and InAs/GaSb, has resulted in several recent theoretical studies of these electron-phonon resonances in SLs\textsuperscript{9,10,11,12,13,14}. Unfortunately, to our knowledge, electron-phonon resonances have not been observed experimentally in SL transport within the NDC regime.

Several choices are available to calculate SL transport in the high and low field regimes. Wacker and Jauho\textsuperscript{15} established the relationship in some cases between different transport calculation methods, including miniband conduction\textsuperscript{1}, Wannier-Stark hopping\textsuperscript{16}, sequential tunnelling\textsuperscript{17}, and the non-equilibrium Green’s function (NGF) formalism\textsuperscript{18} and their respective ranges of validity, and reached the conclusion that the NGF contains the other three as limiting cases. For example, the semiclassical Boltzmann transport equation (BTE), which can be solved to any desired degree of numerical accuracy by Monte Carlo simulations\textsuperscript{19}, cannot accurately describe transport under high-field ($eF L \sim \hbar \omega_0$) conditions\textsuperscript{14,20}. Use of the generalized Kadanoff-Baym(GKB) ansatz\textsuperscript{18,21,22} is limited in validity to slowly varying fields and time dependence.
Rott, Linder and Döhler employed the Wannier-Stark hopping transport technique to study the temperature dependence of electron-phonon resonances. Their method is only applicable to the high-field regime. Emin and Hart obtained a $\delta-$function electron-phonon resonance in the limit of a very wide energy band $\Delta \to \infty$. Bryksin and Kleinert focused on narrow band ($\Delta \to 0$) transport in a one-dimensional NGF model with and without the GKB ansatz. The approximations made in Ref. included relying on the periodic nature of the Green’s functions in a large homogeneous field and discarding the Fourier components of the Dyson equations beyond lowest order. The impurities were modeled with $\delta$-function potentials (and hence only depended on the product of the impurity density and the scattering potential), and the SL bandwidths considered were much smaller than optical phonon energies, in order to obtain analytic expressions for the field-dependent DOS and the transport.

In our treatment here we use the Kadanoff-Baym-Keldysh NGF technique to calculate the non-linear quantum transport. We solve for the field-dependent Green’s functions equations numerically, non-perturbatively including the elastic impurity scattering by directly inverting the NGF Dyson equations. These Green’s functions, and the resulting density of states (DOS), depend on the impurity size, strength, and density separately. We then calculate the effect of inelastic (phonon) scattering as a perturbation. Specifically we leave the retarded Green’s function obtained for elastic scattering unchanged, but alter the less-than Green’s function. A related model, where impurity scattering was treated exactly within the resonant level model, and phonon scattering was treated perturbatively, has been introduced before. In Ref. the analysis focused on comparison of the model results with those obtained from the GKB ansatz. In our treatment we consider more general impurity types, and use the solvability of the model to explore the influence of impurity nature on the electron-phonon resonances. The resulting $I-V$ curves illuminate the nature of the electron-phonon resonances in a regime where elastic scattering dominates.

Because we treat more of the problem numerically we are able to consider all significant Fourier components of the Dyson equation, general SL bandwidths and impurity potential size and strength. In this way we can explore the properties of these electron-phonon resonances for a wider range of parameters with confidence. Our approach therefore possesses several advantages over earlier ones: (i) it employs a more realistic form for impurity potentials that leads to better approximations for the DOS; (ii) other common approximations
are relaxed, including restrictions on the growth axis miniband width; (iii) it is applicable to both high and low field transport; and (iv) it does not use the generalized Kadanoff-Baym ansatz to solve the Dyson equation.

The outline of the paper is as follows. In Sec. II, we show the detailed theoretical and numerical methods used to calculate the retarded and lesser Green’s functions, from which are extracted the DOS and carrier distribution functions. In Sec. III the field dependence of the calculated drift velocity is discussed in detail. We focus on the electron-phonon resonance peaks and the influence of impurity scattering and establish a relationship between earlier results and ours. Our results are discussed and summarized in Sec. IV.

II. THEORY AND NUMERICAL METHOD

A. High-field Green’s function

In order to study high-field effects, we must use an approach that is non-perturbative in the electric field. We consider the scalar potential gauge \( \phi(r,t) = -r \cdot F \), where \( F \) is the time-independent uniform electric field. In the absence of scattering, the Dyson equation of the retarded Green’s function in the \( k \) representation can be written as:

\[
\left[ i\hbar \frac{\partial}{\partial t} - \varepsilon(k) + ieF \cdot \nabla_k \right] G^r_{\phi}(k, t, k', t') = (2\pi)^3 \delta(k - k')\delta(t - t').
\]  

(2.1)

We make use of a 14-band superlattice \( \mathbf{K} \cdot \mathbf{p} \) calculation to obtain the superlattice energy dispersion relations \( \varepsilon(k) \). Only the lowest conduction band with growth-axis width \( \Delta \) is considered in the present transport calculations. We assume the electric field is along the superlattice growth direction (noted as \( || \), and the in-plane directions are noted as \( \perp \)) The \( \mathbf{K} \cdot \mathbf{p} \) results are then fit to a dispersion relation of the form

\[
\varepsilon(k) = \frac{\hbar^2 k^2}{2m^*} + \frac{\Delta}{2} \left[ 1 - \cos(k_{||}L) \right],
\]  

(2.2)

where \( m^* \) is the electron effective mass along the in-plane directions. Solving Eq. (2.1), we get the retarded Green’s function with no scattering

\[
G^r_{\phi}(k_{||}, k'_{||}, k_{\perp}, k'_{\perp}, t - t') = -i(2\pi)^3 \delta \left[ \hbar(k_{||} - k'_{||}) - eF(t - t') \right] \delta(k_{\perp} - k'_{\perp}) \theta(t - t') \\
\times e^{-i \left\{ \left( \frac{\hbar k^2}{2m^*} + \frac{\Delta}{2} \right) (t - t') + \frac{\Delta}{2\pi L} \left[ \sin(k_{||}L) - \sin(k'_{||}L) \right] \right\}}.
\]  

(2.3)
After taking the Fourier transformation \((t - t' \rightarrow \omega)\),

\[
G_r^\phi (k_\parallel, k'_\parallel, k_\perp, k'_\perp,\omega) = -\frac{i(2\pi)^3}{eF} \delta(k_\perp - k'_\perp) \theta(k_\parallel - k'_\parallel)
\times e^{-\frac{1}{4} \left\{ \left( -\omega + \frac{\hbar^2 k_\perp^2}{2m^*} + \hbar^2 \frac{\Delta}{\pi} \sin(k_\parallel L) - \sin(k'_\parallel L) \right) \right\} }.
\]

(2.4)

The corresponding gauge invariant spectral function is

\[
A(k,\omega) = i \left[ G_r^\phi (k,\omega) - G^a (k,\omega) \right]
\]

\[
= 2\pi \sum_{n=-\infty}^{\infty} J_n \left[ -\frac{\Delta}{eF L} \cos(k_\parallel L) \right] \delta \left( \hbar \omega - \frac{\hbar^2 k_\perp^2}{2m^*} - \frac{\Delta}{2} - neF L \right).
\]

(2.5)

The spectral function satisfies the sum rule \((\hbar/2\pi) \int d\omega A(k,\omega) = 1\). The density of states is

\[
\rho(k_\perp,\omega) = \int_{-\pi/L}^{\pi/L} \frac{dk_\parallel}{2\pi} A(k,\omega)
\]

\[
= \frac{2\pi}{L} \sum_{n=-\infty}^{\infty} J_n^2 \left( -\frac{\Delta}{2eF L} \right) \delta \left( \hbar \omega - \frac{\hbar^2 k_\perp^2}{2m^*} - \frac{\Delta}{2} - neF L \right).
\]

(2.6)

The energy of the Wannier-Stark level \(n\) superlattice cells away is \(neF L\). A level with index \(n\) can contribute to the DOS if the miniband width \(\Delta\) is big enough, and its contribution is proportional to \(J_n^2 \left( -\frac{\Delta}{2eF L} \right)\). This result coincides with Wacker’s results based on Wannier-Stark bands\(^{15}\). In the NGF approach of Bryksin\(^{11}\) the terms with \(n > 0\) vanish because the approximation \(\Delta \rightarrow 0\) is used.

B. Elastic impurity scattering and \(G^r\)

For a single impurity at \(\mathbf{R}\), the Dyson equation for the retarded Green’s function is

\[
G_R^r (\mathbf{k}, \mathbf{k}', \omega) = G^\phi (\mathbf{k}, \mathbf{k}', \omega) + \int \frac{d^3\mathbf{q}_1}{(2\pi)^3} \int \frac{d^3\mathbf{q}_2}{(2\pi)^3} G^\phi (\mathbf{k}, \mathbf{q}_1, \omega)
\times e^{-i(\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{R}} V(\mathbf{q}_1, \mathbf{q}_2, \omega) G_R^r (\mathbf{q}_2, \mathbf{k}', \omega).
\]

(2.7)

For elastic impurity scattering, we have \(V(\mathbf{q}_1, \mathbf{q}_2, \omega) = V(\mathbf{q}_1 - \mathbf{q}_2)\). In our calculations, we consider a one-dimension system and use a Gaussian impurity potential with range \(a\) along the growth direction

\[
V(\mathbf{r}_1 - \mathbf{r}_2) = V_0 e^{-\frac{(r_1 - r_2)^2}{a^2}}.
\]

(2.8)

The Fourier transform of the impurity potential is

\[
V(\mathbf{q}_1 - \mathbf{q}_2) = V_0 (2\pi)^2 a \sqrt{\pi} \delta(\mathbf{q}_{1\perp} - \mathbf{q}_{2\perp}) e^{-a^2 (q_{1\parallel} - q_{2\parallel})^2 / 4}.
\]

(2.9)
Omitting the perpendicular component \( \mathbf{k}_\perp, \mathbf{q}_\perp \), we find for the Dyson equation

\[
G^r_R \left( \mathbf{k}_\parallel, \mathbf{k}'_\parallel, \omega \right) = G^r_\phi \left( \mathbf{k}_\parallel, \mathbf{k}'_\parallel, \omega \right) + \int \frac{dq_\parallel}{2\pi} \int \frac{dq'_\parallel}{2\pi} G^r_\phi \left( \mathbf{k}_\parallel, q_\parallel, \omega \right) \\
\times e^{-i(q_\parallel - q'_\parallel)R} V(q_\parallel - q'_\parallel) G^r_R \left( q_\parallel, \mathbf{k}'_\parallel, \omega \right).
\]

(2.10)

The above Green’s function is for only one impurity at site \( R \) and for a single scattering event. When all scattering events at that site are included, the Green’s function and corresponding T-matrix are

\[
G^r_R \left( \mathbf{k}_\parallel, \mathbf{k}'_\parallel, \omega \right) = G^r_\phi \left( \mathbf{k}_\parallel, \mathbf{k}'_\parallel, \omega \right) + \int \frac{dq_\parallel}{2\pi} \int \frac{dq'_\parallel}{2\pi} G^r_\phi \left( \mathbf{k}_\parallel, q_\parallel, \omega \right) \times T'_R \left( q_\parallel, q'_\parallel, \omega \right) G^r_R \left( q'_\parallel, \mathbf{k}'_\parallel, \omega \right),
\]

(2.11)

\[
T'_R \left( q_\parallel, q'_\parallel, \omega \right) = e^{-i(q_\parallel - q'_\parallel)R} V(q_\parallel - q'_\parallel) + \int \frac{dp_\parallel}{2\pi} \int \frac{dp'_\parallel}{2\pi} V(q_\parallel - p_\parallel) \\
\times e^{-i(q_\parallel - p_\parallel)R} G^r_\phi \left( p_\parallel, p'_\parallel, \omega \right) T'_R \left( p'_\parallel, q'_\parallel, \omega \right).
\]

(2.12)

We assume the impurity density is sufficiently dilute that we can approximate the self energy by its impurity-averaged form. The self energy is then

\[
\Sigma^r \left( q_\parallel, q'_\parallel, \omega \right) = c \int dR T_R \left( q_\parallel, q'_\parallel, \omega \right),
\]

(2.13)

where \( c \) is the line concentration of impurities. \( T_R \) differs from \( T'_R \) of Eq. (2.12); we apply the self-consistent Born approximation\(^{23,27}\) and we replace \( G^r_\phi \) (no scattering) in Eq. (2.11) by \( G^r \) (including scattering) to obtain \( T_R \). We find

\[
T_R \left( q_\parallel, q'_\parallel, \omega \right) = e^{-i(q_\parallel - q'_\parallel)R} V(q_\parallel - q'_\parallel) + \int \frac{dp_\parallel}{2\pi} \int \frac{dp'_\parallel}{2\pi} V(q_\parallel - p_\parallel) \\
\times e^{-i(q_\parallel - p_\parallel)R} G^r \left( p_\parallel, p'_\parallel, \omega \right) T_R \left( p'_\parallel, q'_\parallel, \omega \right).
\]

(2.14)

The final Dyson equation for the retarded Green’s function \( G^r \) is thus

\[
G^r \left( k_\parallel, k'_\parallel, \omega \right) = G^r_\phi \left( k_\parallel, k'_\parallel, \omega \right) + \int \frac{dq_\parallel}{2\pi} \int \frac{dq'_\parallel}{2\pi} G^r_\phi \left( k_\parallel, q_\parallel, \omega \right) \times \Sigma^r \left( q_\parallel, q'_\parallel, \omega \right) G^r \left( q'_\parallel, k'_\parallel, \omega \right).
\]

(2.15)

Similar equations for the resonant level model (RLM) were obtained by Jauho\(^{23}\). Here our approach is rather different. Instead of exploring the relationship of these equations to the Boltzmann equation\(^{23}\), we plan to apply the equation numerically to investigate in detail electron-phonon resonances.
Eqs. (2.14) and (2.15) form a closed set of integral equations. In our numerical method, we use a uniformly distributed grid for k-space and R-space integration, hence the double integral becomes a product of matrices. The sizes of these matrices $G^r$ and $T_R$ are typically $600 \times 600$ (15 Brillouin zones and 40 points per zone). The R-space integration in Eq. (2.13) involves about 500 points with a 1000Å grid spacing. To solve the equation set, we first use $G^r_\phi$ as an initial guess for $G^r$ and perform the iteration to obtain a self-consistent solution. Sometimes the iterative process does not converge, in which case we adjust the initial retarded Green’s function, matrix size, or (k,R)-space integral mesh.

C. Polar optical phonon scattering and $G^<$

We assume phonon scattering is very weak compare to elastic scattering. In this limit the Wannier-Stark level broadening is mainly governed by elastic impurity scattering — thus the densities of states are determined by the elastic impurity scattering. We obtain the retarded Green’s function, which determines the DOS, by the procedure of Sec. II B (neglecting phonon scattering). The approach to $G^<$ must be different, however, for this function describes the carrier dynamics. When only elastic impurity scattering is considered, $G^<= -G^r = -1/2[G^r - G^a] = iA/2$, and the net current vanishes. In order to obtain a non-zero current, phonon scattering must be taken into account in $G^<$.

We evaluate the lesser Green’s function directly from the Keldysh equation [18], but with a perturbative approach.

$$G^< = (1 + G^r \Sigma^r)G^<_0(1 + \Sigma^a G^a) + G^r \Sigma^< G^a,$$

(2.16)

where the double momentum labels for each of the Green’s functions and self-energies are implicit and all the products in the equation imply integration over the adjacent momentum label. Here $G^<_0$ is the lesser Green’s function without scattering and is equal to $-[G^r_\phi - G^a_\phi]/2 = iA(k, \omega)/2$. The spectral function neglecting scattering, $A(k, \omega)$ (Eq.(2.5)), has several poles of the form $\delta(E - E_n)$. Scattering makes the poles move away from these energies $E_n$; the first term in Eq. (2.16) is proportional to $(G^r_0)^{-1}G^<_0(G^a_0)^{-1} \propto (E - E_n)^2\delta(E - E_n)$ near the former singular points. As a consequence, the first term in Eq. (2.16) will vanish, so Eq. (2.16) simplifies to

$$G^< = G^r \Sigma^< G^a.$$

(2.17)
Here the self energy is $\Sigma = \Sigma_{\text{imp}} + \Sigma_{\text{pho}}$. Based on analytic continuation, the self energy for impurity scattering is

$$\Sigma_{\text{imp}} = c \int dRT_R^r G^<_T T_R^a. \quad (2.18)$$

For polar optical phonon scattering, the corresponding self energy is expressed as

$$\Sigma_{\text{pho}} = \int \frac{dq}{2\pi} M_q^2 \left[ n_B G^<_T (\omega - \omega_q) + (n_B + 1) G^<_T (\omega + \omega_q) \right], \quad (2.19)$$

where $M_q$ is the electron-phonon coupling matrix element, here treated as a constant, and $n_B = 1/\left\{ \exp[\hbar \omega_q/(k_B T)] - 1 \right\}$ is the Bose-Einstein occupation factor for LO phonons. The frequency of the LO phonons $\omega_q$ is also treated as a constant. The temperature we use is 77K. Earlier work shows higher temperatures will strongly depress the electron-phonon resonances.

The following symmetry holds when there is only elastic scattering: $G(k, k', \omega + \omega_0) = e^{i(k-k') \hbar \omega_0 / \hbar} G(k, k', \omega)$ or alternately $G(k, k', t, t') = G(k, t-t') \delta[k-k'-\frac{eF}{\hbar}(t-t')]$. We assume this symmetry is still present when phonon scattering is included as a perturbation. As a first order approximation, we replace $G^<$ in Eqs. (2.18) and (2.19) with $\frac{i}{2} A_{\text{imp}} = -\frac{1}{2} [G^r_{\text{imp}} - G^a_{\text{imp}}]$. The lesser Green’s function of Eq. (2.17) then becomes

$$G^< = G^r_{\text{imp}} \left[ \Sigma^<_T + \Sigma^<_T \right] G^a_{\text{imp}}$$

$$= G^r_{\text{imp}} \left\{ c \int dRT_R^r \frac{i}{2} A_{\text{imp}} T_R^a \right. + \int \frac{dq}{2\pi} M_q^2 \left[ n_B \frac{i}{2} A_{\text{imp}} (\omega - \omega_q) + (n_B + 1) A_{\text{imp}} (\omega + \omega_q) \right] \} G^a_{\text{imp}}$$

$$= \frac{i}{2} A_{\text{imp}} + G^r_{\text{imp}} \left\{ \int \frac{dq}{2\pi} M_q^2 \left[ \frac{i}{2} n_B e^{-i(k-k') \hbar \omega_0 / \hbar} A_{\text{imp}} (\omega) 
+ \frac{i}{2} (n_B + 1) e^{i(k-k') \hbar \omega_0 / \hbar} A_{\text{imp}} (\omega) \right] \} G^a_{\text{imp}}. \quad (2.20)$$

The first term has been simplified because $iA_{\text{imp}}$ is a solution for the equation $G^<_T = G^r_{\text{imp}} \left[ c \int dRT_R^r G^<_T T_R^a \right] G^a_{\text{imp}}$. The variables on the right side of Eq. (2.20) are all known, so $G^<(k, k', \omega)$ can be found. The current density $J$ depends on $G^<$ according to

$$J = e \int_{-\pi/L}^{\pi/L} \frac{dk}{2\pi} \left[ (-i) G^<(k, t = 0) \frac{1}{\hbar} \frac{\partial \varepsilon(k)}{\partial k} \right]. \quad (2.21)$$
III. RESULTS

A. Impurity scattering effects on electron-phonon resonance

We expect the properties of the electron-phonon resonances to depend significantly on the relative magnitudes of the growth axis bandwidth of the lowest conduction miniband and the optical phonon energy. If the bandwidth $\Delta$ is very large compared to the optical phonon energy, then the electron-phonon resonances can be well described within a Wannier-Stark hopping picture, whereas in the other limit the electron-phonon resonances are better described within a sequential tunnelling picture. We present here detailed results for the drift velocity as a function of electric field for two superlattices, one in each regime.

The first superlattice consists of 12 monolayers of GaAs and 6 monolayers of AlAs (unit cell length 50.9\,Å). The resulting width of the lowest miniband is 20.3\,meV. We use the value for the GaAs optical phonon energy ($\hbar\omega = 36\,\text{meV}$) for this GaAs/AlAs SL, so the ratio of the bandwidth to the optical phonon energy $\Delta/\hbar\omega = 0.56$. The other structure is 7 monolayers of InAs and 12 monolayers of GaSb (unit cell length 57.8\,Å), which has a very broad lowest conduction miniband width of 150\,meV. The optical phonon energy of InAs ($\hbar\omega = 30\,\text{meV}$) is used for the InAs/GaSb superlattice, and hence $\Delta/\hbar\omega = 5$. In both cases, the zone center gap between the lowest and second-lowest minibands is larger than 350\,meV. Thus, the occupation of higher minibands is very small and we can neglect conduction from higher minibands and interminiband Zener tunneling. For convenience in our comparison we approximate the period for the two types of superlattices with the same value, $L = 57\,\text{Å}$.

We have numerically calculated the drift velocity for fields near the electron-phonon resonance value $neFL = \hbar\omega$, which typically ranges from $0.1 \times 10^7$ V/m to $1.0 \times 10^7$ V/m. Because we treat phonon scattering as a perturbation, the calculated drift velocity is directly proportional to the electron-phonon coupling coefficient $M_q^2$. We choose the coupling constant to make the drift velocity realistic ($\sim 10^3\text{m/s}$). To be consistent, the calculated effective relaxation time $\tau_{\text{eff}}$ from phonon scattering should be longer than the relaxation time from impurity scattering: $\tau_{\text{eff}} > 10\,\text{ps}$.

In Fig. 1(a), we show how the density of impurities affects the electron-phonon resonance peaks in the narrow bandwidth superlattice, and in Fig. 1(b) results for the broad bandwidth one. The line concentration of impurities ranges from $1/(464\,\text{Å})$ (defined as $c$ in Fig. 1)
to $1/(58\text{Å})$. These values correspond to $1.0 \times 10^{16}\text{cm}^{-3}$ and $5.1 \times 10^{18}\text{cm}^{-3}$, respectively, in 3-dimensions. We see that large impurity densities will produce weaker electron-phonon resonance peaks. When the impurity density is $4c$, there is only one peak in the velocity-field curve for the broad bandwidth SL (Fig. 1(b)). Indeed, the position of the peak is not at a resonance, so it’s not an electron-phonon resonance at all. Instead, it’s the maximum of the entire velocity-field curve, which is the starting point of NDC. In Fig. 1(a), all the electron-phonon resonance peaks are located in the NDC region. In Fig. 1(b), when the impurity scattering is very strong the electric field corresponding to the maximum current enters the region of our interest. This peak flattens the electron-phonon resonance peaks. The calculated DOS, instead of exhibiting Wannier-Stark levels, is closer to a zero-field DOS.

In Fig. 2, the solid lines show the DOS for different impurity concentrations under the same electric field $F = 0.2 \times 10^7\text{V/m}$ in broad-band superlattice. The DOS for a low impurity density ($c=1/(464\text{Å})$, thin line in the Fig. 2) clearly shows the Wannier-Stark levels. But the DOS for a higher impurity concentration ($c=1/(116\text{Å})$, thick line) tends to be very similar to the zero-field result (which is shown as the dashed line). Properly approaching the zero-field DOS and the appearance of the maximum of current in the velocity-field curves indicate our method is valid for low-field situations. This contrasts with the Wannier-Stark hopping method that is often used in high-field transport, which will diverge under low-field conditions$^{12,15}$.

In Fig. 3, we compare the effects of the impurity strength $V_0$ and impurity density $c$ on the electron-phonon resonances. We find that the impurity strength can diminish the drift velocity considerably, but does not affect the height of the electron-phonon resonances as much as the concentration of impurities does. In Fig. 4, we change the impurity size but keep $V_0a$ fixed to observe changes in the electron-phonon resonances. When the impurity size increases, the resonance becomes weaker.

Figs. 3 and 4 are calculated results for relatively perfect materials. We also model more imperfect materials by employing an impurity density of $1/(19\text{Å})$ (corresponding to $1.46 \times 10^{20}\text{cm}^{-3}$ in three dimensions), and use a rather small value for the impurity strength $V_0$. The impurity size produces different effects on the electron-phonon resonance peaks for different bandwidths. In Fig. 5(a), for the narrow bandwidth SL, impurities of larger size (with $V_0a$ constant) flatten the electron-phonon resonance peaks. This contrasts with Fig. 5(b), for the broad bandwidth SL, where larger impurities enhance the electron-phonon resonances

"enhance"
stronger. This phenomena can be explained by comparing with the one-dimensional square potential barrier scattering problem. The reflection coefficient of a scattering electron is not a monotonic function of the barrier size (still keeping $V_0a$ constant)\(^{28}\). Instead, there is a maximum value for the reflection probability. We take $\Delta/2$ as the average energy of incoming electrons and calculate the impurity size that maximizes the reflection coefficient. For the narrow bandwidth SL, $a_{\text{max}} = 11.3\text{Å}$, whereas for the broad bandwidth SL, $a_{\text{max}} = 1.5\text{Å}$. Hence impurity scattering generates different trends for narrow and broad bandwidth SLs in the region $2\text{Å} < a < 8\text{Å}$.

There is another feature distinguishing relatively clean and dirty superlattices. In the clean case the electron-phonon resonance in the narrow bandwidth SL is stronger than in broad bandwidth one. But in the dirty case, the electron-phonon resonance in the narrow bandwidth SL is weaker than in the broad bandwidth one, e.g. when the impurity size is $a = 8\text{Å}$. The reason for this is as follows: when $V_0a$ is large, all the collisions between electrons and impurities are essentially total reflection. In this case, impurity scattering in a broad bandwidth SL is stronger than in a narrow bandwidth one because the spatial extent of the Wannier-Stark wave function $\Delta/eF$ is proportional to the bandwidth $\Delta$. Thus electrons in a broad bandwidth SL experience more collisions in a Wannier-Stark oscillation period. But when $V_0a$ is small, the collisions have both substantial transmission and reflection. The incoming electrons in a broad bandwidth SL have more energy and a larger transmission coefficient than in a narrow bandwidth SL. This makes impurity scattering in broad bandwidth SLs weaker than in narrow bandwidth ones, which is the opposite of the clean case.

\section*{B. Comparison with earlier results}

We have also reproduced the earlier work of Bryksin and Kleinert\(^{11}\) and find a relation between Bryksin’s parameter for impurity scattering and ours: $h\sqrt{U} \approx V_0\sqrt{ac}$. However, this relation has a limited range of applicability because the DOS of a Wannier-Stark level generally does not have the half-elliptical shape employed by Bryksin,

$$\propto 1/(2\pi U)Re\sqrt{4U - \bar{\omega}^2}. \quad (3.1)$$
Fig. 6 shows the DOS for different parameter sets and compares them to Bryksin’s and Wacker’s\cite{14,15} results. When $ac$ is very large, the DOS tends to have a half-elliptical shape. From Fig. 6, we also can see a shift of the DOS. If there is no scattering, the main band is centered at $E = \Delta/2$. Impurity scattering will shift all bands to higher energies. When $ac$ is big enough the shape of the DOS is Bryksin-like and the energy shift has the form $E_{\text{center}} = E_{0\text{center}} + \delta E = \Delta/2 + \sqrt{\pi V_0 ac}$. Bryksin’s DOS centers on the zero-energy point because they used $\Delta \to 0$. Wacker’s DOS also remains centered on the point $E = 0$ because they chose localized Wannier-Stark states as the basis of the wave function, as have many others\cite{27}. Wacker’s DOS also uses the approximation of a constant scattering self-energy,

$$G^r(E, k_\perp) = \sum_n \frac{J_n^2(\Delta/2eFL)}{E - neFL - E_{k_\perp} + (i\Gamma/2)}, \quad (3.2)$$

where $-i\Gamma/2$ is the self-energy (in Fig. 6 we adopt $\Gamma = 2h\sqrt{U}$). The shape of Wannier-Stark state using a constant self-energy is not realistic. However, Eq. (3.2) does produce the appropriate side band. Bryksin’s DOS uses the miniband approximation $\Delta/2eFL \ll 1$ and neglects the side band, and therefore obtains a field-independent DOS. For the narrow-band SL, $\Delta = 20\text{meV}$, the central band occupies $J_0^2(\Delta/2eFL) = 90.7\%$ of the entire density when a typical electric field $F = 0.4 \times 10^7 V/m$ is used.

In Fig. 7, we reproduce Bryksin’s velocity-field curve using a very large value for $ac$. The agreement is very good. When $ac$ is small, the DOS deviates from the half-elliptical shape and becomes asymmetric. The asymmetry manifests in a low energy side which has a larger density than the high energy side [see Fig. 6(a)]. For a realistic superlattice, $ac < 1$, so the half-elliptical shape will typically not exist.

We have also calculated the approximate momentum relaxation times ($\tau$) for different impurity parameters and present them in Table 1. The $\tau$’s are calculated by fitting the retarded Green’s function $|G^r(k, t)|$ to an exponential decay $e^{-t/\tau}$. In Bryksin’s limit (using the half-elliptical DOS), $G^r(t)$ has the form $J_1(2\sqrt{Ut})/\sqrt{Ut}$, which oscillates in time and exhibits a power-law decay. In our calculations, the decay of $G^r$ is neither Bryksin-like nor exponential. The decay of $G^r(t)$ is Bryksin-like when $t$ is short, and the decay is exponential when $t$ is long. In the intermediate region, the decay displays a complex shape that depends on the specific impurity scattering parameters.
IV. DISCUSSION

The advantages of our computational method are: (i) we treat realistic scattering strengths and obtain a realistic DOS; (ii) many common approximations are relaxed, such as the small bandwidth ($\Delta \to 0$), the high-field ($\Omega \tau_{\text{eff}} \gg 1$) and the relaxation time approximations; (iii) compared to the Wannier-Stark hopping method that was mainly used under high-field conditions, our method is applicable to both high and low field transport; and (iv) we do not use the generalized Kadanoff-Baym ansatz\textsuperscript{18} to solve the Dyson equation.

In our calculations, we used the approximation that phonon scattering is weak compared to impurity scattering. It is straightforward in principle to eliminate this approximation in the non-equilibrium Green’s function method by adding self-energy terms for phonon scattering $\Sigma_{\text{pho}}^{\text{r}}$ to Eq. (2.15).

$$
\Sigma_{\text{pho}}^{\text{r}} = \int \frac{dq}{2\pi} \frac{M_q^2}{q} \left[ n_B G^r (\omega - \omega_q) + (n_B + 1) G^r (\omega + \omega_q) \right]
$$

\footnotesize{$$
+i \int \frac{d\omega'}{2\pi} G^< (\omega - \omega') \left( \frac{1}{\omega' - \omega_0 + i0^+} - \frac{1}{\omega' + \omega_0 + i0^+} \right) .
$$}

If we ignore the last term in Eq. (4.1), which corresponds to a low carrier concentration approximation, then Eq. (2.15) is a closed equation for the retarded Green’s function. Based on the retarded Green’s function, we can use iteration or some other method to solve the Quantum Kinetic Equation (2.17) to obtain the lesser Green’s function. If the low carrier concentration approximation is relaxed, Eq. (2.15) and Eq. (2.17) are coupled and more iterations are needed. In the both cases, the computational effort is much greater than the present approach.

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Table 1. Calculated approximate relaxation times for different impurity scattering strengths.

| Impurity parameters | Approximate relaxation time(ps) |
|---------------------|---------------------------------|
|                     | $\Delta = 20\text{meV}$ | $\Delta = 150\text{meV}$ |
| $a(\text{Å})$ | $V_0(\text{eV})$ | $c(1/\text{Å})$ | | |
| 20 | 0.1 | 1/464 | 8.95 | 1.73 |
| 20 | 0.1 | 2/464 | 3.09 | 0.377 |
| 20 | 0.1 | 4/464 | 0.905 | 0.116 |
| 20 | 0.1 | 8/464 | 0.470 | — |
| 100 | 0.02 | 1/464 | 3.32 | 1.18 |
| 100 | 0.04 | 1/464 | 2.12 | 0.683 |
| 100 | 0.02 | 2/464 | 0.940 | 0.321 |
Figure captions

Figure 1: Drift velocity versus field for different impurity concentration (a) in a narrow band superlattice ($\Delta = 20\text{meV}$) and (b) in a broad band superlattice ($\Delta = 150\text{meV}$). The unit of impurity concentration $c = 1/(464\text{Å})$. Inset of (a) shows a clear view of the velocity-field curves for the high impurity densities $4c$ and $8c$ because the drift velocity is very small. The impurity scattering strength $V_0 = 0.1\text{eV}$, and the impurity size $a = 20\text{Å}$.

Figure 2: The calculated DOS for different impurity concentrations for the broad band-width superlattice ($\Delta = 150\text{mV}$). $c = 1/(464\text{Å})$ and the electric field $F$ is in units of $10^7\text{V/m}$. The zero-field DOS is shown for comparison (dashed line).

Figure 3: Different effects of impurity strength and concentration on electron-phonon resonance peaks in a (a) narrow bandwidth and (b) broad bandwidth superlattice. The parameters used are $c = 1/(464\text{Å})$, $V_0 = 0.02\text{eV}$, and $a = 100\text{Å}$.

Figure 4: velocity-field curves for different impurity sizes with a fixed $V_0a (= 2\text{eV} \cdot \text{Å})$ in a (a) narrow bandwidth and (b) broad bandwidth superlattice. The impurity concentration $c=1/(464\text{Å})$.

Figure 5: The drift velocity-field relations for different impurity sizes while $V_0a$ keeps constant ($= 0.12\text{eV} \cdot \text{Å})$ in (a) narrow bandwidth and (b) broad bandwidth superlattices. The impurity density $c = 1/(19\text{Å})$.

Figure 6: (a) calculated DOS for different $ac$, for $V_0\sqrt{ac} = \text{const.}(1.7\text{meV})$, (b) Bryksin-type DOS ($h\sqrt{U} = 1.7\text{meV}$); and Wacker-type DOS, with a constant self-energy $\Gamma/2 = h\sqrt{U} = 1.7\text{meV}$.

Figure 7: Reproduction of Bryksin’s results for two bandwidths ($\Delta = 20\text{meV}$, $36\text{meV}$). Bryksin’s parameter $h\sqrt{U} = 1.7\text{meV}$. Our parameters are $V_0 = 0.425\text{meV}$ and $ac = 16$. 

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FIG. 1: Shaoxin Feng et al.
FIG. 2: Shaoxin Feng et al.
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FIG. 7: Shaoxin Feng et al.