Defect capturing and charging dynamics and their effects on magneto-transport of electrons in quantum wells

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Abstract
The calculated defect corrections to the polarization and dielectric functions for Bloch electrons in quantum wells are presented. These results were employed to derive the first two moment equations from the Boltzmann transport theory and then applied to explore the role played by defects on the magneto-transport of Bloch electrons. Additionally, we have derived analytically the inverse momentum-relaxation time and mobility tensor for Bloch electrons by making use of the screened defect-corrected polarization function. Based on quantum-statistical theory, we have investigated the defect capture and charging dynamics by employing a parameterized physics-based model for defects to obtain defect wave functions. Both capture and relaxation rates, as well as the density for captured Bloch electrons, were calculated self-consistently as functions of temperature, doping density and chosen defect parameters. By applying the energy-balance equation, the number of occupied energy levels and the chemical potential of defects were determined, with which the transition rate for defect capturing was obtained. By applying these results, the defect energy-relaxation, capture and escape rates, and Bloch-electron chemical potential were calculated self-consistently for a non-canonical subsystem of Bloch electrons. At the same time, the energy- and momentum-relaxation rates of Bloch electrons, as well as the current suppression factor, were also investigated quantitatively. By combining all these results, the temperature dependence of the Hall and longitudinal mobilities was presented for Bloch electrons in either single- or multi-quantum wells.

Keywords: defect capturing, charging dynamics, magneto-transport, quantum wells, energy balance, energy-relaxation

(Some figures may appear in colour only in the online journal)
1. Introduction

Point defects can strongly affect the physical properties of materials and have a significant impact on their performance in devices. Spectroscopy based on positron annihilation proves itself particularly suitable for studying vacancy-type defects in semiconductors [1]. Sometimes, point defects appear to dominate both physical and chemical properties of semiconductors, and their characterization based on experimental techniques alone is often found insufficient. In these situations, one needs combining experiment and theory studies to gain a full picture for the interaction dynamics of point defects with electrons [2]. First-principles density functional theory computations [3, 4] are proved as an effective approach that complements experiments as a predictive tool in identifying and characterizing defects. A general thermodynamic formalism [4, 5], on the other hand, can also be established for studying the physical properties of thermal-equilibrium point defects. Recently, the vibrational spectroscopy demonstrates itself as an alternative approach for identifying defects and determining their microscopic structures and dynamics in crystals [6]. Meanwhile, point defects and impurities are found theoretically to strongly affect both optical and transport properties of semiconductor materials [7].

In the past, defect studies have heavily focus on material point and extended defects which are formed during a crystal-growth process. In contrast with these crystal-growth defects, for space environment, we concentrate our attention on proton-generated point defects (vacancies, interstitials and voids) in semiconductors. These are attributed to displacements of atoms from their thermal-equilibrium lattice sites [8, 9]. In this case, the lattice-atom displacements do not result from crystal growth but are caused by a proton-irradiation-induced primary knock-on atom for building up point defects before their reactions. Such atom displacements depend not only on the energy-dependent flux of protons but also on the differential energy transfer cross sections (or probabilities) for collision between atoms, interatomic Coulomb interactions and even kinetic-energy loss to core-level electrons of an atom (e.g., ionizations). One of the effective calculation methods for studying the non-thermal spatial-temporal distributions of proton-induced point defects is the molecular-dynamics model [10]. For non-equilibrium interaction dynamics between conduction electrons and point defects, however, only very few of the self-consistent microscopic-level models have been proposed for systematically investigating the defect dynamical effects based on a many-body theory [11] beyond the thermal-equilibrium density-functional theory, including transition rate, charging, capture, relaxation, scattering and current suppression.

Dangling bonds attached to point defects are capable of capturing Bloch electrons by emitting multi-phonons to form localized charged centers. The resulting randomly distributed charge centers modify electron responses to either an external ballistic electron beam [12] or incident photons [13]. The influence due to defects on the electronic response function can be taken into account by a vertex correction [13] to a bare polarization function for non-interacting electrons within the ladder approximation (LA) [14]. On the other hand, the screening effect due to electron–electron interactions on this bare polarization function can be included by employing the random-phase approximation (RPA) [14]. The quantum-statistical theory presented in this paper is crucial for fully understanding the mechanism involved in characterizing the defect species [15] and defect effects [16]. Aided by our present microscopic theory for non-equilibrium interaction dynamics of point defects, the experimental characterization of irradiated test devices [17–19] is able to provide more useful information on the device architecture’s susceptibility to space radiation effects [20]. By studying non-equilibrium dynamics of interacting point defects with conduction electrons, numerical results for both capture and relaxation times, as well as self-consistent captured electron density for a non-canonical system of only conduction electrons, can be calculated as functions of the lattice temperature, doped electron density and chosen defect parameters. The relationship between our theory and experimental measurements includes, e.g., the defect capture time versus decayed photoluminescence peak with time, and current-suppression factor versus the reduced photocurrent in post-irradiated detectors. For possible advantages of our theory, we would like to point out that it could help the design of quantum-well focal plane arrays [21, 22] which must be characterized in advance for damages by space radiation [23, 24]. They should achieve not only high performance [25] but also radiation tolerance to the radiation encountered in a satellite orbit.

The rest of the paper is organized as follows. In section 2, by employing an extended point-defect wave function, we present our theoretical model to investigate effects of interaction between point defects and conduction electrons on the polarization and dielectric functions of quantum wells. We obtain the first two moments from Boltzmann transport equation (BTE) in section 3 which are in turn used to determine the dynamical role played by defects in quantum-well magneto-transport. In section 4, we calculate the inverse momentum-relaxation time and mobility tensor by using the defect-corrected polarization function for electron magneto-transport. By going beyond a simple $\delta$-function for point-defect probability function, we study in section 5 the non-equilibrium capture and charging dynamics for point defects and obtain the capture and relaxation rates, as well as the density of captured subband electrons as well in a self-consistent approach. A brief summary is given in section 6 along with some remarks.

2. Defect effect on polarization function

In our previous work, we have used a static point-scattering model with a $\delta$-function for the defect spatial probability distribution and a fixed charge number in its interaction with conduction electrons. In this paper, we instead introduced a new parameterized quantum mechanical model for point vacancies by employing a finite-range probability function with assumed binding energies and binding radii for various types of defects. Consequently, the interaction between point defects and conduction electrons will be modified by a
nonlocal form factor, depending on the transition wave number of electrons and point-defect location. Meanwhile, we have also introduced an effective charge number, which is dependent on both temperature and defect Fermi energy determined by an energy-balance equation for the total number of bound electrons accommodated by a point defect. In this way, the single-particle Coulomb interaction between a charged point defect and a conduction electron will rely uniquely on the temperature and defect Fermi energy. Furthermore, a new formalism, using the frequency-derivative of a defect-corrected polarization function, has been established in this paper for computing inverse momentum-relaxation time of electrons in quantum wells. For this reason, we will review and retain some related formalism established in our previous work while highlighting the new physics involved in our present extended dynamical scattering model for Coulomb interaction between a point defect and conduction electrons in quantum wells.

Since the spatial range for the wave functions of individual defects is very much limited, we anticipate that the interaction between electrons and charged defects can only affect the screening of the intralayer Coulomb interaction between electrons. Therefore, we begin with the effects arising from defect in a single quantum well. The theoretical study on exchange-interaction function of electrons in a quantum well has been previously reported [13] within the LA. Recently, the defect-induced vertex correction to a bare polarization function in electrons in a quantum well has been previously reported [13] within the LA. Recently, the defect-induced vertex correction to a bare polarization function in electrons in quantum-multi-wells has also been investigated [7].

For a single narrow quantum well, the separation between two adjacent conduction subbands is large, and at low density only the lowest subband will be occupied by electrons (i.e., electric-quantum limit). In this case, the screened electron polarization function \( \chi_{\parallel}^{(0)}(q_{\parallel}, \omega) \) can be calculated with the use of an inverse dielectric function \( \epsilon^{-1}(q_{\parallel}, \omega) \), according to [12]

\[
\chi_{\parallel}^{(0)}(q_{\parallel}, \omega) = \epsilon^{-1}(q_{\parallel}, \omega) \chi_{\parallel}^{(0)}(q_{\parallel}, \omega) \Gamma(q_{\parallel}, \omega),
\]

where \( \Gamma(q_{\parallel}, \omega) \) represents an intra-well defect-vertex correction, which can be determined by equation (8) below, and the bare polarization function \( \chi_{\parallel}^{(0)}(q_{\parallel}, \omega) \) takes the form [7]

\[
\chi_{\parallel}^{(0)}(q_{\parallel}, \omega) = \frac{1}{2\pi} \int_{0}^{2\pi} dk_{\parallel} \int_{0}^{2\pi} dk_{\perp} \frac{1}{q_{\parallel}^{2} + \frac{\hbar^{2}}{m^{*}} k_{\parallel}^{2}} \times \left[ f_{0}(\varepsilon_{k_{\parallel}} - u_{0}) - f_{0}(\varepsilon_{k_{\parallel} + q_{\parallel}} - u_{0}) \right] \times \text{Re} \left[ \frac{1}{\hbar \omega - \imath \gamma_{0} - \varepsilon_{k_{\parallel} + q_{\parallel}} + \varepsilon_{k_{\parallel}}} \right] + \imath \pi L_{0} \left( \hbar \omega - \varepsilon_{k_{\parallel} + q_{\parallel}} + \varepsilon_{k_{\parallel}}, \gamma_{0} \right),
\]

where \( L_{0}(a, b) = (b/\pi)/(a^{2} + b^{2}) \) is the Lorentz shape function, \( \phi_{k_{\parallel}, q_{\parallel}} \) is the angle between wave vectors \( k_{\parallel} \) and \( q_{\parallel} \), \( \gamma_{0} \) is the energy-level broadening, \( \varepsilon_{k_{\parallel}} = \hbar^{2} k_{\parallel}^{2}/2m^{*} \) is the subband kinetic energy, \( m^{*} \) is the effective mass, \( f_{0}(x) = [1 + \exp(x/k_{B}T)]^{-1} \) is the Fermi function for thermal-equilibrium electrons, \( u_{0} \) and \( T \) are the chemical potential (evaluated from the subband edge) and temperature of electrons (or lattice phonons), respectively.

Additionally, for a single occupied subband, the inverse dielectric function \( \epsilon(q_{\parallel}, \omega) \) employed in equation (1) is simply given by \( \epsilon(q_{\parallel}, \omega) = 1/\epsilon_{q_{\parallel}}^{\parallel}(\omega) \), where \( \epsilon_{q_{\parallel}}^{\parallel}(\omega) \) is the dielectric function of electrons and is calculated [14] within the RPA as

\[
\epsilon(q_{\parallel}, \omega) = 1 - v_{e}(q_{\parallel}) \chi_{1}^{(0)}(q_{\parallel}, \omega) \Gamma(q_{\parallel}, \omega),
\]

and the second term in equation (3) contains the defect-vertex correction \( \Gamma(q_{\parallel}, \omega) \) to the polarization function. In equation (3), \( v_{e}(q_{\parallel}) \) represents the intra-well Coulomb interaction between pair of electrons, given by [7]

\[
v_{e}(q_{\parallel}) = \frac{e^{2}}{2\pi\epsilon_{0}q_{\parallel}} \int_{0}^{\infty} dk_{\parallel} \int_{-\infty}^{\infty} dz \left[ \frac{\partial f_{0}(\varepsilon_{k_{\parallel}} - u_{0})}{\partial \varepsilon_{k_{\parallel}}} \right],
\]

which plays the role of the inverse of static screening length [7].

For the defect-vertex correction, \( \Gamma(q_{\parallel}, \omega) \), introduced in equations (1) and (3), we find the following self-consistent equation within the LA [7]

\[
\Gamma(q_{\parallel}, \omega) = 1 + \frac{1}{2\pi^{2}} \int_{0}^{\infty} dp_{\parallel} p_{\parallel}^{2} \chi_{1}^{(0)}(p_{\parallel}, \omega) \Gamma(p_{\parallel}, \omega)
\]

\[
\times \delta(\varepsilon_{q_{\parallel}}^{\parallel} - \varepsilon_{p_{\parallel}}^{\parallel}) \int_{-\ell_{0}/2}^{\ell_{0}/2} d\xi \rho_{d}(\xi)
\]

\[
\times \int_{0}^{\pi} d\phi_{q_{\parallel}, p_{\parallel}} |U_{d}(q_{\parallel}, p_{\parallel}, T, \xi)|^{2}
\]

\[
= 1 + \frac{2m^{*}}{\pi^{2} \hbar^{2}} \chi_{1}^{(0)}(q_{\parallel}, \omega) \Gamma(q_{\parallel}, \omega)
\]

\[
\times \int_{-\ell_{0}/2}^{\ell_{0}/2} d\xi \rho_{d}(\xi) |\tilde{U}_{d}(q_{\parallel}, T, \xi)|^{2},
\]

where \( \phi_{q_{\parallel}, p_{\parallel}} \) is the angle between two wave vectors \( q_{\parallel} \) and \( p_{\parallel} \), and from equation (C10) the defect interaction \( |\tilde{U}_{d}(q_{\parallel}, T, \xi)|^{2} \)
with electrons is calculated as
\[
\left| \mathcal{T}_d(q_j, T, \xi) \right|^2 \equiv \int_0^\pi d\phi \left| U_d(q_j, p_j, T, \xi) \right|^2_{|q_j|=p_j} = \left( a_0 / a_d \right)^2 \frac{Z_{\text{eff}}(T, E^*) \epsilon^2}{2\epsilon_0 \epsilon_r} \times \int_0^\pi d\phi \left( e^{-\Delta_0(q_j, \phi) \lambda_j^*/2} \times \int_0^\infty dz \int_{-\infty}^{\infty} dz' \left( |\phi_F(z)|^2 \left( e^{-\Delta_0(q_j, \phi) |z-z'|} + e^{-\Delta_0(q_j, \phi) |z+z'|} \right) Q_1(\Delta_0(q_j, \phi), \xi - \xi) \right)^2 \right),
\]
(7)

where \( a = 2 \ell_0 \) is the unit-cell size of a single well, \( a \) is the interwell separation, \( \Delta_0(q_j, \phi) = q_j |\sin(\phi/2)|, \) and \( \lambda_j \) is the correlation length for randomly-distributed defects. Here, different from using a fixed charge number in reference [7], \( Z_{\text{eff}}(T, E^*) \) in equation (7) stands for a one-dimensional density distribution of defects to vacancies with a point-vacancy small radius \( a_0 \), which leads to a lot of occupied lower energy levels and then a very large value for \( Z_{\text{eff}}(T, E^*) \). Furthermore, \( \rho_{\text{tot}}(\xi) \) in equation (6) stands for a one-dimensional density distribution of defects to be determined by defect generation and diffusion [7] under proton radiation. Although the defect states are static, the occupation of these defect states is dynamical, which is determined by interaction between point defects and conduction electrons in the system.

The lowest-order approximate solution of equation (6) can be obtained simply by replacing \( \Gamma(q_j, \omega) \) with 1 on the right-hand side of this equation. Therefore, the leading correction to \( \Gamma(q_j, \omega) \approx 1 \) becomes proportional to the total number of defects or integral of \( \rho_{\text{tot}}(\xi) \left| \mathcal{T}_d(q_j, T, \xi) \right|^2 \) with respect to \( \xi \). In general, the exact solution of equation (6) includes all the higher orders of the integral of \( \rho_{\text{tot}}(\xi) \left| \mathcal{T}_d(q_j, T, \xi) \right|^2 \) by going beyond the second-order Born Approximation [26].

Based on the calculated \( \left| \mathcal{T}_d(q_j, T, \xi) \right|^2 \) in equation (7), equation (6) can be applied to compute the dynamical defect-vertex correction \( \Gamma(q_j, \omega) \) with respect to unity within the LA. In order to simulate the physical distribution of defects due to proton radiation [7], we assume in this paper a regional form [7], i.e., \( \rho_{\text{tot}}(\xi) = \rho_0 \Theta(-\xi - \ell_0) + \rho_0 \Theta(\xi - \ell_0) + [\rho_W + \xi (\Delta\rho/2\ell_0)] \Theta(\ell_0 - |\xi|), \) where \( \Theta(x) \) is a unit-step function, \( \kappa_0 \) is a scaling factor, and \( \rho_W, \rho_L, \rho_R, \Delta\rho \) are parameters for linear defect densities in different regions of a quantum well. Equation (6) can be solved exactly and we are able to find the scattering resonance from the peak in the density plot of
\[
\Gamma(q_j, \omega) = \left[ 1 - \frac{2m^*}{\pi \epsilon_r \epsilon_0} \chi_0(0, \omega) \int d\xi \rho_{\text{tot}}(\xi) \right]^{-1/2} \times \left| \mathcal{T}_d(q_j, T, \xi) \right|^2
\]
within the \((\omega, q_j)\)-plane. The strength of this scattering resonance decreases rapidly with increasing \( q_j \) due to reduced \( \left| \mathcal{T}_d(q_j, T, \xi) \right|^2 \) from the suppressed long-range scattering but increases with \( \kappa_0 \) nonlinearly.

The calculated \( \Gamma(q_j, \omega) \) can be substituted into equation (3) to obtain the intra-well RPA dielectric function modified by defects. In the absence of defects, we will find one intrasubband-plasmon mode and one particle–hole continuum (i.e., \( \text{Im}[\chi_0(0, \omega)] \neq 0 \)), corresponding, for a single occupied subband in a quantum well [7]. After introducing defects to the quantum well, the dispersion of this plasmon mode will be modified for small \( q_j \) values due to an energy shift from the contribution of \( \text{Re}[\Gamma(q_j, \omega)] \). Such a modification to the plasmon dispersion can acquire a nonlinear \( \kappa_0 \) dependence for large \( \kappa_0 \) values (or higher defect densities).

For a multi-quantum-well system, on the other hand, its density–density response function \( \chi_{\lambda,f}(q_j, \omega) \) satisfies the following self-consistent dynamical equation [12]
\[
\chi_{\lambda,f}(q_j, \omega) = \chi_1(q_j, \omega) \delta_{\lambda,f} + \chi_1(q_j, \omega) \times \sum_{j'=(\nu+j=1)}^N \nu_{\lambda}(j, j' | q_j) \chi_{f',f}(q_j, \omega),
\]
(9)
where the integers \( j = 0, 1, \ldots, N \) label \( N + 1 \) different quantum wells, the summation over \( j' \) excludes the intra-well term with \( j' = j \), and the single-layer \( \chi_1(q_j, \omega) \) is determined from equation (1). Moreover, the inter-well Coulomb coupling \( \nu_{\lambda}(z, z' | q_j) \) between two electrons in equation (9), including the image potentials, is calculated as [12]
\[
\nu_{\lambda}(z, z' | q_j) = \frac{\beta_0(q_j) e^2}{2\epsilon_0 \epsilon_r(n_j | q_j) + q_j} \left[ e^{-|q_j - z'|} + \alpha_0 e^{-2q_j |z'-z'|} \right]
\]
\[+ \alpha_0 e^{-q_j |z+z'|} + \alpha_0 e^{-2q_j |z-z'|} \]
(10)
where \( L_{\text{tot}} = N \ell_0, \alpha_0 = \frac{\alpha_0}{\epsilon_0 \epsilon_r}, \) and \( \beta_0(q_j) = \left[ 1 - \alpha_0 \exp(-2q_j L_{\text{tot}}) \right]^{-1}. \) By using the calculated density–density response function \( \chi_{\lambda,f}(q_j, \omega) \) in equation (9), we are able to find the optical conductivity [27] and the inverse momentum-relaxation time as well as in section 4.
3. Magneto-transport in a quantum well

For an n-doped semiconductor quantum well, we begin with the well-known semi-classical BTE \([28–30]\) for conduction electrons within the lowest subband \(\varepsilon_1\) in the electric-quantum limit. BTE has been widely used for different electron transports in various semiconductors and other materials, including covalent materials \([31]\), dilute alloys \([32]\), graphene and novel two-dimensional (2D) materials \([33]\). For our current case, under the condition \(\Delta E_{n,k} \gg \hbar \omega\), the non-equilibrium conduction electron distribution function \(f(r_1,k_1; t)\) in position-momentum space satisfies \([34]\)

\[
\frac{\partial f(r_1,k_1; t)}{\partial t} + \left(\frac{d\mathbf{r}_1(t)}{dt}\right)_{av} \cdot \nabla_{\mathbf{r}_1} f(r_1,k_1; t) + \left(\frac{d\mathbf{k}_1(t)}{dt}\right)_{av} \cdot \nabla_{\mathbf{k}_1} f(r_1,k_1; t)
\]

\[
= \frac{\partial f(r_1,k_1; t)}{\partial t} \bigg|_{coll} - 2 \sum_{n=1}^{\infty} n^2 T_n(k_1, T)
\]

\[
\times \left\{ f(r_1,k_1; t) (1 - P_n) - \left[ 1 - f(r_1,k_1; t) \right] P_n e^{-\Delta E_{n,k}/k_B T} \right\}
\]

\[
\approx \frac{\partial f(r_1,k_1; t)}{\partial t} \bigg|_{coll} = \mathcal{R}_c(k_1, T, E^*) f(r_1,k_1; t),
\]

where \(r_1\) is a 2D position vector, \(k_1\) is a 2D wave vector, the first term at the right-hand side of the above equation represents the collision contributions of electrons with defects, phonons and other electrons, \(\Delta E_{n,k} = \hbar \omega / 2 + |\varepsilon_k| + |E_n|, E_n\) is the defect nth energy level, \(P_n\) the defect nth energy-level non-equilibrium occupation function, and the last step only holds for \(k_B T \ll \Delta E_{n,k}\). Moreover, \(T_n(k_1, T)\) in equation (11) stands for the transition rate which has been calculated in equations (36) and (41). Here, the conduction-electron capture rate \(\mathcal{R}_c(k_1, T, E^*)\) introduced in the last term of equation (11) is computed according to

\[
\mathcal{R}_c(k_1, T, E^*) = 2 \sum_{n=1}^{\infty} n^2 T_n(k_1, T) \left[ 1 - f_0(E_n - E^*) \right].
\]

Furthermore, for subband electrons, we can define, in a semi-classical way, their group velocity through \(\langle d\mathbf{r}_1(t)/dt \rangle_{av} \equiv v(k_1) = (1/\hbar) \nabla_{\mathbf{k}_1} \varepsilon_{k_1}\). Finally, we introduce the semi-classical-Newton-type force equation for the wave vector of subband electrons, yielding

\[
\hbar \left( \frac{d\mathbf{k}_1(t)}{dt} \right)_{av} \equiv F(k_1, t) = -e \left[ E(t) + v(k_1) \times \mathbf{B}(t) \right],
\]

where \(E(t)\) and \(B(t)\) are the external transient electric and magnetic fields, respectively, while \(F(k_1, t)\) represents a microscopic electro-magnetic force acting on a drift electron in the \(k_1\) state.

Based on equation (11), one acquires the zeroth-order moment of BTE by summing over all the \(k_1\) states on both sides of this equation. This directly leads to the generalized electron number conservation law, i.e.,

\[
\frac{\partial n_0(r_1, t)}{\partial t} + \nabla_{r_1} \cdot \mathbf{J}_c(k_1, t) = -\mathcal{R}_c(T, u_0, E^*) \rho_c(r_1, t),
\]

where the electron areal density \(\rho_c(r_1, t)\), the sheet current density \(\mathbf{J}_c(r_1, t)\) and the electron–density capture rate \(\mathcal{R}_c(T, u_0, E^*) \rho_c(r_1, t)\) are defined respectively by

\[
\rho_0(r_1, t) = \frac{2}{A} \sum_{k_1} f(r_1,k_1; t),
\]

\[
\mathbf{J}_c(r_1, t) = \frac{2}{A} \sum_{k_1} v(k_1) f(r_1,k_1; t),
\]

\[
\mathcal{R}_c(T, u_0, E^*) \rho_c(r_1, t) = \frac{2}{\rho_0(u_0) A} \sum_{k_1} \mathcal{R}_c(k_1, T, E^*)
\]

\[
\times \left\{ f(r_1,k_1; t) - f_0(\varepsilon_{k_1} - u_0) \right\},
\]

\[
\rho_0(u_0) = N_c / A, N_c\ is the total number of subband electrons in the system (not conserved due to captured electrons by defects), \(A\) is the quantum-well cross-sectional area, the spin-degeneracy of electrons is included, and \(\mathcal{R}_c(T, u_0, E^*)\) represents average of the capture rate.

For the first-order moment of BTE, however, we have to employ the so-called Fermi kinetics \([34]\). Therefore, we first introduce the relaxation-time approximation (RTA) for subband-electron collisions, which conserves the total subband-electron number and is given by

\[
\frac{\partial f(r_1,k_1; t)}{\partial t} \bigg|_{coll} = \frac{\langle f(r_1,k_1; t) - f_0(\varepsilon_{k_1} - u_0) \rangle}{\tau_\varepsilon(k_1)},
\]

where \(\tau_\varepsilon(k_1)\) describes the total energy-relaxation time for electrons in the \(k_1\) state, including electron–electron, electron–phonon and electron–defect interactions. After a time longer than the defect relaxation and capture times (see section 5), the chemical potential \(u_0(T)\) of the subband-electron system can be determined self-consistently from

\[
N_c = \frac{2}{A} \sum_{k_1} f_0(\varepsilon_{k_1} - u_0) = \int d^2 \mathbf{r}_1 \rho(r_1, t)
\]

\[
= \frac{2}{A} \sum_{k_1} \int d^2 \mathbf{r}_1 f(r_1,k_1; t).
\]

Finally, by applying the RTA to the BTE in equation (11), we find

\[
f(r_1,k_1; t) + \tau_\varepsilon(T, u_0) \frac{\partial f(r_1,k_1; t)}{\partial t}
\]

\[
+ \tau_\chi(T, u_0) \mathcal{R}_c(k_1, T, E^*) f(r_1,k_1; t)
\]
equation (23) can be formally written as

\[
\tau_0(T, u_0) \cdot \nabla \kappa, f_0(\varepsilon_k) - u_0) = 0
\]

where we have assumed that both \( T \) and \( u_0 \) are spatially uniform throughout the system. Additionally, \( \tau_0(T, u_0) \) introduced in the above equation represents average of the energy-relaxation time, yielding

\[
\frac{1}{\tau_0(T, u_0)} \approx \frac{2}{N_e} \sum_{k_i} f_0(\varepsilon_{k_i} - u_0) \frac{1}{\tau_0(k_i)}
\]

where we have neglected the intrinsic contributions from Coulomb (for low electron densities) and phonons (for low temperatures) scattering in doped semiconductors, and \( \tau_0(k_i) \) is attributed to the extrinsic scattering between electrons and defects. The explicit expression for \( \tau_0(k_i) \) can be found from equation (A1).

Now, let us further introduce an inverse momentum-relaxation time tensor \( \tau_p^{-1} \) in connection with equation (13).

For this purpose, we would like to employ first the so-called force-balance equation [34, 35] for a transient macroscopic drift velocity \( v_0(t) \) under external electric and magnetic fields, \( E(t) \) and \( B(t) \), giving rise to

\[
\frac{dv_0(t)}{dt} = -\tau_p^{-1} \cdot v_0(t) + \frac{\mathcal{M}^{-1}}{e} \cdot F_e(t)
\]

\[
= -\tau_p^{-1} \cdot v_0(t) - e\mathcal{M}^{-1} \cdot [E(t) + v_0(t) \times B(t)] = 0
\]

where \( F_e(t) = -e [E(t) + v_0(t) \times B(t)] \) is the macroscopic electromagnetic-force, while the statistically-averaged inverse effective-mass tensor \( \mathcal{M}^{-1} \) for isotropic subband is

\[
\mathcal{M}^{-1}_{ij} = \frac{2}{N_e \hbar^2} \sum_{k_i} \left( \frac{\partial^2 \varepsilon_{k_i}}{\partial k_i \partial k_j} \right) f_0(\varepsilon_{k_i} - u_0)
\]

\[
= \delta_{ij} \frac{2}{N_e \hbar^2} \sum_{k_i} \left( \frac{\partial^2 \varepsilon_{k_i}}{\partial^2 k_i} \right) f_0(\varepsilon_{k_i} - u_0).
\]

The explicit form for \( \tau_p^{-1} \) in the system will be presented in section 4 next. As shown in appendix B, the solution of equation (23) can be formally written as

\[
v_0(t) = \hat{\mu}[B(t)] \cdot E(t),
\]

where \( \hat{\mu}[B(t)] \) is the so-called mobility tensor [34] for describing magneto-transport of subband electrons, which also depends on \( \tau_p^{-1} \) and \( \mathcal{M}^{-1} \) in addition to \( B(t) \). The details for calculating \( \hat{\mu}[B(t)] \) can be found in appendix B. Using equations (23) and (25), we are able to simply rewrite the macroscopic electro-magnetic force as \( F_e(t) = \left( \mathcal{M} \otimes \tau_p^{-1} \right) \cdot [\hat{\mu}[B(t)] \cdot E(t)] \), where \( \mathcal{M} \) represents the inverse of the tensor \( \mathcal{M}^{-1} \).

In a similar way with deriving equation (14), multiplying both sides of equation (21) by the group velocity \( v(k_i) \) and summing over all the \( k_i \) states afterwards, we arrive at

\[
[1 + s_c(T, u_0, E')] J_0(t) + \tau_0(T, u_0) \frac{dJ_0(t)}{dt} = -\tau_0(T, u_0) \frac{2}{A} \sum_{k_i} v(k_i) \left[ F_e(t) \cdot v(k_i) \right]
\]

\[
\times \frac{\partial f_0(\varepsilon_{k_i} - u_0)}{\partial \varepsilon_{k_i}}
\]

\[
= \tau_0(T, u_0) \frac{2}{A} \sum_{k_i} v(k_i) \left\{ \left[ \mathcal{M} \otimes \tau_p^{-1} \right] \cdot [\hat{\mu}[B(t)] \cdot E(t)] \right\} \cdot v(k_i)
\]

\[
\times \left[ \frac{\partial f_0(\varepsilon_{k_i} - u_0)}{\partial \varepsilon_{k_i}} \right],
\]

where the first term on the left-hand side of this equation includes the captured sheet current density \( s_c(T, u_0, E') J_0(t), \) \( s_c(T, u_0, E') = \bar{R}_{\text{int}} \) and \( \tau_0(T, u_0, E') \) is the current-suppression factor (historically also called the current-capture probability if \( s_c(T, u_0, E') \ll 1 \), and the second term on the left-hand side of the equation represents the non-adiabatic correction to \( J_0(t) \), e.g., \( dJ_0(t)/dt = -i \omega J_0(t) \) if \( E(t) = E_0 e^{-i \omega t} \) is assumed. From equation (26) we know that the number current density \( J_0 \) is independent of \( r_j \) within the RTE. Consequently, from equation (14) we find that the number areal density \( \rho_0 \) remains to be a constant \( \rho_0(\varepsilon_i) \) after a time longer than the defect energy-relaxation and capture times, and is determined by

\[
\rho_0(\varepsilon_i) = n_{\text{dop}} - \rho_{\text{cap}}(T, u_0, E') = \frac{2}{A} \sum_{k_i} f_0(\varepsilon_{k_i} - u_0) \equiv \frac{N_e}{A},
\]

which should determine self-consistently the chemical potential \( \varepsilon_i(T) \) of the system at any given \( T \). In equation (27), \( n_{\text{dop}} \) is the given extrinsic areal doping density, \( E' \) the Fermi energy for bound electrons inside thermal-equilibrium defects, and \( \rho_{\text{cap}}(T, u_0, E') \) represents the captured areal electron density as calculated by equation (48). For the subsystem containing conduction electrons only, it is not a canonical system since \( N_e \) will change with time as long as the defect-capturing process is still going on. However, the whole system containing both conduction electrons and point defects remains as a canonical system.

If the external fields are static, i.e., \( E_0 \) and \( B_0 \), we get the sheet charge current density \( f_0 \equiv -eJ_0 \) from equation (26),
i.e.,
\[ j_0 = -\frac{e\tau_0(T, u_0)}{1 + s(T, u_0, E^*)} \frac{2}{\cal A} \sum_{k_i} \nu(k_i) \times \left\{ \left[ \hat{\mathcal{M}} \otimes \hat{\tau}_p^{-1} \right] \cdot \left[ \frac{\nu(B_0)}{E_0} \right] \right\} \cdot \nu(k_i) \times \left[ -\frac{\partial f_0(\varepsilon_{k_i} - u_0)}{\partial \varepsilon_{k_i}} \right]. \]  

(28)

In this case, the elements of a conductivity tensor \( \sigma(B_0) \) can be obtained through the relation \( \sigma_i(B_0) = \frac{\hbar \nu_i}{k_0 e^2} \), where \( i, j = x, y, \) and \( e_\perp, \) \( e_\parallel \) are two unit vectors in 2D position space. From equation (28), we further find that the conductivity tensor depends not only on the mobility tensor, but also how electrons are thermally-distributed within a subband.

As a special case, we consider an isotropic parabolic subband written as \( \varepsilon_{k_i} = \hbar^2 k_i^2/2m^* \), we find from equation (24) that \( \mathcal{M}_{ij} = (1/m^*) \delta_{ij}, \mathcal{M}_{ij} = m^* \delta_{ij}, \) and \( \left[ \hat{\tau}_p^{-1} \right]_{ij} = (1/\tau_p) \delta_{ij}. \) In this case, from equation (B12) we get the mobility tensor
\[ \left[ \hat{\sigma}(B_0) \right]_{ij} = -\frac{\mu_0}{1 + \mu_0^2 B_i^2} \left[ \frac{1}{\mu_0 B_i} - \mu_0 B_i \right], \]  

(29)

where \( \mu_0 = \pi \tau_p / m^* \) for \( E_0 = \{ E_x, E_y, 0 \} \) and \( B_0 = \{ 0, 0, B_z \}. \) If we further assume \( B_0 = 0, \) equation (29) simply reduces to \( \mu_{ij} = -\mu_0 \delta_{ij}. \) In this case, from equation (28) we recover the well-known Ohm’s law \( j_0 = (\pi \mu_0^2 \tau_p / m^*)E_0 \) after setting \( s(T, u_0, E^*) = 0, \) which implies \( \sigma_{ij} = (\pi \mu_0^2 \tau_p / m^*) \delta_{ij}. \)

4. Momentum dissipation from defect scattering

The inverse momentum-relaxation-time tensor \( \hat{\tau}_p^{-1} \), first introduced in equation (23), comes from an average resistive forces \( \mathcal{F}_p \) due to elastic scattering of electrons with randomly-distributed defects in a quantum well [34].

For field-driven electrons moving with a drift velocity \( \nu_d \), the total resistive force \( \mathcal{F}_p \), which can be evaluated from elastic momentum dissipation due to defect elastic scattering, is calculated in the quasi-elastic limit as [34]

\[ \mathcal{F}_p = -\frac{2\pi N_d}{\hbar A^2} \sum_{k_i | q_i} h q_i \left( h q_i \cdot (\nu_d) \right) |U_0(q_i)|^2 \left( -\frac{\partial f_{k_i}}{\partial \varepsilon_{k_i}} \right) \times \delta(\varepsilon_{k_i + q_i} - \varepsilon_{k_i} + h q_i \cdot \nu_d), \]  

(30)

where \( N_d \) is the total number of defects, and

\[ |U_0(q_i)|^2 = \left( \frac{m^*}{2\pi \hbar^2} \right)^{2} Z_{0d}(T, E^*) \frac{2}{2\pi e_\perp} \left[ \frac{e^{-q_i^2/2}}{q_i + \iota} \right]^2 \times \int_{0}^{\Lambda_0/2} d\zeta_0 \rho_0(\xi) \left[ \int_{-\infty}^{\infty} dz_0 \int_{-\infty}^{\infty} dz_0' |\mathcal{F}_0(z)|^2 \right] \times \left( e^{\frac{q_i |z - \iota|}{2}} + e^{\frac{-q_i |z - \iota|}{2}} \right). \]

(31)

Here, for simplicity we have introduced the notation \( f_{k_i} \equiv f_0(\varepsilon_{k_i} - u_0) \) in equation (30). Using the relation \( \hat{\tau}_p^{-1} \cdot \nu_d = -\frac{1}{\hbar N_d} \hat{\mathcal{M}}^{-1} \cdot \mathcal{F}_p, \) as obtained from the force-balance equation in equation (23), we get from equation (30) the inverse momentum-relaxation-time tensor \( \hat{\tau}_p^{-1} \) in the quasi-elastic limit, yielding
\[
\frac{1}{\hat{\tau}_p^{-1}} \cdot \nu_d = \frac{4\pi \hbar \sigma_d}{\rho_0(u_0) A^2} \sum_{k_i | q_i} \left[ U_0(q_i) \right]^2 \left( -\frac{\partial f_{k_i}}{\partial \varepsilon_{k_i}} \right) \times \delta(\varepsilon_{k_i + q_i} - \varepsilon_{k_i} + h q_i \cdot \nu_d) \left\{ \hat{\mathcal{M}}^{-1} \otimes \left[ q_i \otimes q_i^* \right] \right\},
\]

(32)

where \( \sigma_d = N_d / A \) is the point-defect areal density, and the \( 2 \times 2 \) matrix is defined as
\[
\left[ q_i \otimes q_i^* \right] \equiv \left[ q_i^2 \ q_i q_i^* \ q_i q_i^* \ q_i^2 \right].
\]

Finally, by employing the expression in equation (2) and the density–density response function \( \chi_{jj}(q_i, \omega) \), determined from equation (9), we can rewrite equation (30) in a compact form, i.e.,
\[
\mathcal{F}_p = \frac{N_d}{A} \sum_{q_i} |U_0(q_i)|^2 \Im \left\{ \chi(q_i, \omega) = -q_i \cdot \nu_d \right\},
\]

(33)

where we have defined a total density–density response function \( \chi(q_i, \omega) \) for the whole multi-quantum-well system, given by \( \tilde{\chi}(q_i, \omega) = \sum_{k_i=0}^{N} \chi_{jj}(q_i, \omega). \) By using equation (33), the inverse momentum-relaxation-time tensor \( \hat{\tau}_p^{-1} \) presented in equation (32) can also be rewritten in the quasi-elastic limit as
\[
\frac{1}{\hat{\tau}_p^{-1}} \cdot \nu_d = \frac{2\pi \sigma_d}{\rho_0(u_0) A} \sum_{q_i} \left[ U_0(q_i) \right]^2 \left\{ \frac{\partial}{\partial \omega} \Im \left\{ \tilde{\chi}(q_i, \omega) \right\} \right\}_{\omega=0} \times \left\{ \hat{\mathcal{M}}^{-1} \otimes \left[ q_i \otimes q_i^* \right] \right\}.
\]

(34)

Assuming \( \hat{\mathcal{M}}^{-1} = \mathcal{M}_0^{-1} \) with \( \mathcal{M}_0^{-1} \) as a unit matrix, we get from equation (34) that \( \tau_p^{-1} = (1/\tau_p) \mathcal{M}_0^{-1} \) and
\[
\frac{1}{\tau_p} = \frac{\sigma_d}{m^* \rho_0(u_0) A} \sum_{q_i} \left[ U_0(q_i) \right]^2 \left\{ \frac{\partial}{\partial \omega} \Im \left\{ \tilde{\chi}(q_i, \omega) \right\} \right\}_{\omega=0}.
\]

(35)

From the result in equation (35), we are able to calculate the mobility tensor of this multi-quantum-well system using equation (29), which includes the scattering contribution from defects in the system.
By utilizing the Fröhlich Hamiltonian model [42], the electron–phonon coupling matrix element $|\langle \psi_{n,t,m} | U_{ep} | \phi_{k_{\ell}} \rangle |^2$ in equation (36) is evaluated as

$$\left| \langle \psi_{n,t,m} | U_{ep} | \phi_{k_{\ell}} \rangle \right|^2 = e^{\frac{2}{2\epsilon_{\ell} \epsilon_{l}}} \left( \frac{1}{\epsilon_{H} - \epsilon_{L}} \right) h\Omega_{0} \frac{1}{2} (2\pi)^2 \left[ e^{-\frac{2}{\epsilon_{\ell} \epsilon_{l}}} \frac{1}{\epsilon_{H} - \epsilon_{L}} \right] \frac{1}{2} \frac{1}{(2\pi)^2} \times \int d\mathbf{q} \int d\mathbf{z} \int d\mathbf{z}' \left[ e^{-\frac{2}{\epsilon_{\ell} \epsilon_{l}}} \frac{1}{\epsilon_{H} - \epsilon_{L}} \right] F_{0}(\mathbf{z}) \times B_{s,t,m}(\mathbf{q}_{l} + \mathbf{k}_{\ell}, \mathbf{z} - \mathbf{z}') \times F_{r}(\mathbf{z}') \right]. \tag{37}$$

where $\epsilon_{l}$ and $\epsilon_{L}$ are the static and optic dielectric constants of the host semiconductor, while the Fourier-transformed partial form factor $B_{s,t,m}(\mathbf{q}_{l} + \mathbf{k}_{\ell}, \mathbf{z})$ of a defect is

$$B_{s,t,m}(\mathbf{q}_{l} + \mathbf{k}_{\ell}, \mathbf{z}) \equiv \int d\mathbf{r}_{l} \left| \psi_{n,t,m}(\mathbf{r}_{l}, \mathbf{z}) \right| e^{-i\mathbf{q}_{l} \cdot \mathbf{r}_{l}} = \sqrt{2\pi} e^{i\mathbf{q}_{l} \cdot \mathbf{r}_{l}} \int_{0}^{\infty} dr_{l} \mathcal{P}_{l} \int_{0}^{\infty} \frac{dr_{l}'}{\sqrt{r_{l}^2 + z^2}} \times \mathcal{P}_{l} (z/\sqrt{r_{l}^2 + z^2}). \tag{38}$$

In equation (38), $\psi_{n,t,m}(\mathbf{r}_{l}, \mathbf{z})$ has been employed from equation (C3), $J_{m}(x)$ is the first-kind Bessel function of order $m$, and $\theta_{k_{\ell} + \mathbf{q}_{l}} = \tan^{-1}((k_{\ell} + q_{l})/(k_{\ell} + q_{l}'))$ is the angle between the wave vector $\mathbf{k}_{\ell} + \mathbf{q}_{l} = (k_{\ell} + q_{l}, k_{\ell} + q_{l}')$ and positive $x$-axis. Here, the prefactor in front of the integral with respect to $r_{l}$ in equation (38) only contributes a $2\pi$ factor in equation (37).

Based on the calculated transition rate $T_{n}(k_{\ell}, \mathbf{z})$ in equation (36) and thermal-equilibrium energy-level occupation $f_{d}(E_{n} - E)$ in equation (C12), as well as using the defect-relaxation time approximation, we arrive at the following dynamical equation for non-equilibrium occupation $\mathcal{P}_{n}$ of bound electrons on the nth energy level of a defect, i.e.,

$$\left(1 - \mathcal{P}_{n} \right) \frac{2}{\rho_{0}(\mathbf{u}_{0})} \sum_{k_{\ell}} f_{0}(\varepsilon_{k_{\ell}} - u_{0}) T_{n}(k_{\ell}, T) - \mathcal{P}_{n} \frac{2}{\rho_{0}(\mathbf{u}_{0})} \sum_{k_{\ell}} \left[ 1 - f_{0}(\varepsilon_{k_{\ell}} - u_{0}) \right] \times e^{-\frac{\Delta E_{n,k_{\ell}}}{k_{B}T}} T_{n}(k_{\ell}, T) \times \prod_{n' > n} D_{n',\alpha}(T) \mathcal{P}_{n'} - \mathcal{P}_{n} \sum_{n' > n} D_{n',\alpha}(T) (1 - \mathcal{P}_{n'}) \quad + \quad \prod_{n' > n} D_{n',\alpha}(T) \mathcal{P}_{n'} e^{-\frac{E_{n'} - E_{\alpha}}{k_{B}T}} \left(1 - \mathcal{P}_{n} \right) \sum_{n' < n} D_{n',\alpha}(T) \mathcal{P}_{n'} \text{ for } n' < n.$$
where the non-radiative inter-level transition rate $D_{n'n}(T)$ from the $n$th to the $n'$th energy level is

$$ D_{n'n}(T) = \frac{2\pi}{\hbar} \exp \left\{ -[1 + 2N_0(\Omega_0)]S_0 + \frac{|E_n - E_{n'}|}{2k_BT} \right\} \times \left( 1 - \frac{|E_n - E_{n'}|}{\hbar S_0} \right)^2 \sum_{\alpha} \sum_{\ell,f,m} \delta \left( \alpha - \frac{|E_n - E_{n'}|}{\hbar S_0} \right) \sum_{n'\prime} \left| \langle \psi_{n',\ell,m'}(r_1, z)|U_{q\ell}(r_1, z)|\psi_{n,f,m}(r_1, z) \rangle \right|^2 .$$

(40)

In addition, the average rate $T_n(k_j, T, \xi)$ in equation (36) with respect to transition position $\xi$ becomes

$$ T_n(k_j, T) = \frac{1}{N_\xi/2} \int_{-\xi\eta/2}^{\xi\eta/2} d\xi \rho_\xi(\xi) T_n(k_j, T, \xi) .$$

(41)

the $n$th-level defect-relaxation time, $\tau_n^d(T, u_0, E^*)$, is given by

$$ \frac{1}{\tau_n^d(T, u_0, E^*)} = \frac{2}{\rho_0(u_0)A} \sum_{k_j} T_n(k_j, T) \left\{ f_0(\varepsilon_{k_j} - u_0) + \left[ 1 - f_0(\varepsilon_{k_j} - u_0) \right] e^{-\varepsilon_{k_j}/k_BT} \right\} + \frac{1}{\rho_0(u_0)A} \sum_{n' > n} D_{n'n}(T) f_0(E_{n'} - E^*) + \frac{1}{\rho_0(u_0)A} \sum_{n' < n} D_{n'n}(T) f_0(E_{n'} - E^*) \times e^{-|E_n - E_{n'}|/k_BT} + \frac{1}{\rho_0(u_0)A} \sum_{n' \neq n} D_{n'n}(T) \left[ 1 - f_0(E_{n'} - E^*) \right] + \frac{1}{\rho_0(u_0)A} \sum_{n' \neq n} D_{n'n}(T) \left[ 1 - f_0(E_{n'} - E^*) \right] \times e^{-|E_n - E_{n'}|/k_BT} ,$$

(42)

and $N_\xi = \int_{-\xi\eta/2}^{\xi\eta/2} d\xi \rho_\xi(\xi)$ is the total number of defects in a single quantum-well structure. For $k_BT \ll \Delta E_{k_j}$ (i.e., insignificant single-phonon emission regime) and $D_{n'n}(T) \ll T_n(k_j, T)$ (i.e., neglecting much weaker interlevel non-radiative transitions within a defect), equation (42) further leads to a statistically-average defect-relaxation time $\tau_n^d(T, u_0, E^*)$ for all captured electrons inside a defect, given by

$$ \frac{1}{\tau_n^d(T, u_0, E^*)} = \frac{2}{\rho_0(u_0)A} \sum_{n=1}^{\infty} n^2 \rho_n(T, u_0, E^*) \times 2 \sum_{n=1}^{\infty} n^2 \rho_n(T, u_0, E^*) \times \frac{1}{Z_{\text{eff}}(T, E^*)} \sum_{k_j} T_n(k_j, T) \left\{ f_0(\varepsilon_{k_j} - u_0) + \left[ 1 - f_0(\varepsilon_{k_j} - u_0) \right] e^{-\varepsilon_{k_j}/k_BT} \right\} + \frac{1}{\rho_0(u_0)A} \sum_{n' \neq n} D_{n'n}(T) \left[ 1 - f_0(E_{n'} - E^*) \right] + \frac{1}{\rho_0(u_0)A} \sum_{n' \neq n} D_{n'n}(T) \left[ 1 - f_0(E_{n'} - E^*) \right] \times e^{-|E_n - E_{n'}|/k_BT} ,$$

(43)

As a result, we obtain the non-equilibrium occupation function $P_n(T, E^*, u_0)$ for the $n$th energy level of a defect, given by

$$ P_n(T, u_0, E^*) = f_0(E_n - E^*) - \tau_n^d(T, u_0, E^*) \times \frac{2}{\rho_0(u_0)A} \sum_{n=1}^{\infty} n^2 \rho_n(T, u_0, E^*) \times \left[ 1 - f_0(E_n - E^*) \right] + \frac{1}{\rho_0(u_0)A} \sum_{n' \neq n} D_{n'n}(T) \left[ 1 - f_0(E_{n'} - E^*) \right] \times e^{-|E_n - E_{n'}|/k_BT} .$$

(44)

which can be employed for calculating any average physical quantities associated with a defect. Meanwhile, using the calculated $T_n(k_j, T)$ and $f_0(E_n - E^*)$, we obtain the statistically-average capture rate $\gamma_n^{\text{cap}}(T, u_0)$ for subband electrons by the $n$th energy level of a defect, that is,

$$ \gamma_n^{\text{cap}}(T, u_0) = \frac{2}{\rho_0(u_0)A} \sum_{k_j} T_n(k_j, T) f_0(\varepsilon_{k_j} - u_0) .$$

(45)

Again, this gives rise to a statistically-average capture rate $\gamma_n^{\text{cap}}(T, u_0, E^*)$ by a defect, i.e.,

$$ \gamma_n^{\text{cap}}(T, u_0, E^*) = \frac{1}{Z_{\text{eff}}(T, E^*)} \sum_{n=1}^{\infty} n^2 \gamma_n^{\text{cap}}(T, u_0)(1 - P_n) \times \frac{1}{Z_{\text{eff}}(T, E^*)} \sum_{n=1}^{\infty} n^2 \gamma_n^{\text{cap}}(T, u_0)(1 - P_n) \times \left[ 1 - f_0(E_n - E^*) \right] + \frac{2}{\rho_0(u_0)A} \sum_{k_j} T_n(k_j, T) \times f_0(\varepsilon_{k_j} - u_0) .$$

(46)
In a similar way, we also find a statistically-averaged escape rate \( \gamma_{\text{esc}}^d(T, u_0, E^*) \) by a defect, given by

\[
\gamma_{\text{esc}}^d(T, u_0, E^*) \approx \frac{1}{Z_{\text{eff}}(T, E^*)} \sum_{n=1}^{\infty} 2n^2 f_0(E_n - E^*) \times e^{-\Delta E_{nk}/k_B T} \times \frac{2}{\rho(u_0) A} \sum_{k|} T_{\text{d}}(k|, T) \times \left[ 1 - f_0(\xi_{k|} - u_0) \right],
\]

where \( \gamma_{\text{esc}}^d(T, u_0, E^*) \ll \gamma_{\text{cap}}^d(T, u_0, E^*) \) if \( \Delta E_{nk} \gg k_B T \). Finally, from equation (44) we get the density \( \rho_{\text{cap}}(T, u_0, E^*) \) for total captured subband electrons by all defects in a quantum well, yielding

\[
\rho_{\text{cap}}(T, u_0, E^*) = N_\text{d} \left[ \gamma_{\text{esc}}^d(T, u_0, E^*) - \gamma_{\text{cap}}^d(T, u_0, E^*) \right] \rho(u_0)
\]

\[
= N_\text{d} c_{\text{eff}}^d(T, u_0, E^*) \sum_{k|} \frac{1}{Z_{\text{eff}}(T, E^*)} \times \sum_{n=1}^{\infty} 2n^2 T_{\text{d}}(k|, T) \times \left[ f_0(\xi_{k|} - u_0) \right] 
\]

\[
\times \left[ 1 - f_0(E_n - E^*) \right] \left[ 1 - e^{-\Delta E_{nk}/k_B T} \right] - f_0(E_n - E^*) e^{-\Delta E_{nk}/k_B T} \right].
\]

(47)

(48)

By combining equations (46) with (48), the charge-conservation law in equation (27) requires

\[
n_{\text{dop}} \equiv \rho(u_0) + \rho_{\text{cap}}(T, u_0, E^*)
\]

\[
= 2 \sum_{k|} \left( f_0(\xi_{k|} - u_0) \right) + \frac{N_\text{d} c_{\text{eff}}^d(T, u_0, E^*)}{Z_{\text{eff}}(T, E^*)} \sum_{n=1}^{\infty} 2n^2 T_{\text{d}}(k|, T) \times \left[ f_0(\xi_{k|} - u_0) \right] \left[ 1 - f_0(E_n - E^*) \right]
\]

\[
\times \left[ 1 - e^{-\Delta E_{nk}/k_B T} \right] - f_0(E_n - E^*) e^{-\Delta E_{nk}/k_B T} \right],
\]

(49)

from which the chemical potential \( u_0 \) can be computed as the root of equation (49) for any fixed values of \( n_{\text{dop}} \) and \( T \), as well as for \( E^* \) determined from equation (C12).

6. Numerical results and discussions

In our numerical calculations, we have used parameters in table 1. The other parameters are set by: \( L_0 = 2\ell_0 + a = 3\ell_0, \rho_\ell = 3 \times 10^8 \text{ cm}^{-1}, \rho_B = 2.5 \times 10^8 \text{ cm}^{-1}, \rho_W = 1.5 \times 10^8 \text{ cm}^{-1}, \Delta \rho = 1.0 \times 10^9 \text{ cm}^{-1}, \) and \( 1 \leq \kappa_0 \leq 10 \).

Moreover, the units of energy and wave number of electrons are given by \( k_T = \sqrt{2\pi m_0} = 5.6 \times 10^7 \text{ m}^{-1} \) and \( E_T = \hbar^2 k_B^2/2m_0 = 1.8 \text{ meV} \), respectively, for selected areal density \( n_{\text{dop}} = 5 \times 10^{11} \text{ m}^{-2} \). The rest of parameters, such as \( N \) and \( \kappa_0 \), will be given directly in the figure captions.

Our models and theories developed in sections 2 through 5 are microscopic and physics-based, and require no fitting parameters. Consequently, whether or not the theory itself is correct and accurate depends on the physical mechanism and approximation employed. We are aware that only an approximate parabolic dispersion is used for the low kinetic energy of the ground state electrons in quantum wells. Therefore, we are confident that the results presented in this paper are correct, at least qualitatively if not quantitatively. On the other hand, the direct measurement of a calculated microscopic physical quantity in experiments is very challenging if not impossible. The extraction of such a microscopic physical quantity from experimental data usually relies on simulations with a selected physics-based model. Consequently, comparison between results from computations and experiments are definitely nontrivial. Additionally, the other factors in a testing sample, e.g., impurity and interface-roughness scattering, may also play a role in measured transport characteristics. But, we believe that our calculated microscopic physics quantities, as displayed in figures 4 and 5 as functions of temperature \( T \) are still relevant to some experimental observations [2012 Appl. Phys. Lett. 101, 251108; 2015 IEEE Trans. Nucl. Sci. 62, 512], e.g., defect capture time versus decayed photoluminescence peak with time and current-suppression factor versus the reduced photocurrent in post-irradiated detectors.

To display charging dynamics for bound electrons in a void, we display calculated results for \( n^*(E_d, a_d) \) from equation (C12), \( E^*(T, N^*) \) from equation (C15) and \( Z_{\text{eff}}(T, Z^*) \) from equation (C6) in figure 2. Figure 2(a) shows the density plot for number of occupied levels \( n^*(E_d, a_d) \) with respect to defect captured electrons as functions of void binding energy \( E_d \) and binding radius \( a_d \), where separated belts with \( n^* = 2, 3, \ldots, 6 \) are found and \( n^* \) goes up with either \( E_d \) or \( a_d \). The enhancements of \( n^* \) by \( E^* \) and \( a_d \) are associated with higher releasing energy from a defect-capturing process and weakened Coulomb repulsion between bound electrons in the void. Figure 2(b) presents the chemical potential \( E^*(T, N^*) \) as functions of total number \( N^*(E_d, a_d) \) for bound electrons and temperature \( T \), where \( E^* \) is found decreasing with \( T \) due to smearing of Fermi surface for bound electrons but increasing with \( N^* \) due to presence of more bound electrons. To display specific features clearly, we also present \( E^*(T, N^*) \) as a function of \( N^* \) in figure 2(c) with several values of \( T \), where a stepwise enhancement of \( E^* \) by reducing \( T \), as well as by enlarging \( N^* \), show up clearly in figure 2(c). In figure 2(d), we plot the calculated \( E^* \) dependence for effective charge number \( Z_{\text{eff}}(T, E^*) \) at various temperatures, in which the exponential increase of \( Z_{\text{eff}}(T, Z^*) \) with \( E^* \) appears as expected, that is further supplemented by enhanced \( Z_{\text{eff}}(T, Z^*) \) with \( T \) due to thermal excitation of bound electrons to higher-energy levels with much higher orbital degeneracy.
Table 1. Parameters used for numerical calculations.

| Parameter | Description | Value | Units |
|-----------|-------------|-------|-------|
| $\hbar\omega_0$ | Level separation | 75 | meV |
| $m^*$ | Effective mass | 0.067 | $9.1 \times 10^{-31}$ kg |
| $\epsilon_s$ | Static dielectric constant | 12.9 | |
| $\epsilon_L$ | Optic dielectric constant | 10.89 | |
| $\hbar\Omega_0$ | Phonon energy | 36 | meV |
| $\epsilon$ | Dielectric constant | 11.9 | |
| $\Lambda_{\parallel}$ | Correlation length | 10 | nm |
| $\gamma_0$ | Level broadening | 1 | meV |
| $n_{dop}$ | Doping density | 5 | $10^{10}$ cm$^{-2}$ |
| $T$ | Temperature | 300 | K |
| $S_0$ | Huang–Rhys factor [41] | 1.1 | |
| $a_{d}$ | Void binding radius | 10 | nm |
| $a_{0}$ | Point vacancy binding radius | 5 | Å |
| $E_d$ | Defect binding energy | 300 | meV |
| $\sigma_d$ | Point-defect areal density | 5 | $10^9$ cm$^{-2}$ |

*Here, chosen values for listed parameters in the upper part of table correspond to GaAs material, whereas those in the lower part of table were considered in our previous study [43].

Figure 2. (a) Density plot for the number of occupied levels $n^*(E_d, a_d)$, calculated from equation (C12), as functions of void binding energy $E_d$ and binding radius $a_d$. (b) Density plot for the chemical potential $E^*(T, N^*)$ of defect-captured electrons, calculated from equation (C15), as functions of temperature $T$ and total number of captured electrons $N^*$. (c) Plots of $E^*(T, N^*)$ as a function of $N^*$ at different temperatures $T = 150, 200, 250, 300$ K. (d) Logarithm plots of $Z_{\text{eff}}(T, E^*)$, calculated from equation (C6), as a function of $E^*$ at different temperatures $T = 150, 200, 250, 300$ K.

and conduction electrons. From figure 3(a), we find that the transition rate $T_n(k_{\parallel}, T, \xi)$ for conduction electrons to the $n = 1$ ground state of defect decreases with $T$ in the high-$T$ regime (i.e., $N_0(\omega_0) \gg 1$ and $\eta_0 \propto n_0(\Omega_0) \gg 1$) mainly resulting from reduction from the exponential factor $T_n(k_{\parallel}, T, \xi) \propto \exp(\Delta E_{n,k_{\parallel}}/2k_B T)$, due to detailed balance with escaped bound electrons from defect, as $T$ goes up. Meanwhile, $T_n(k_{\parallel}, T, \xi)$ becomes slightly higher for larger values of $k_{\parallel}$, which results from the minor increase of $\Delta E_{n,k_{\parallel}}$ in the same exponential factor $\exp(\Delta E_{n,k_{\parallel}}/2k_B T)$. In addition, $T_n(k_{\parallel}, T, \xi)$ in figure 3(b) drops three-order of magnitude for the $n = 2$ excited state of defect because of significantly decreasing $\Delta E_{n,k_{\parallel}}$ with $n$. On the other hand, for $T_n(k_{\parallel}, T, \xi)$ as functions of $k_{\parallel}$, as shown in figures 3(c) and (d), we observe a rise of the transition rate with $k_{\parallel}$ at $T = 300$ K due to increased $\Delta E_{n,k_{\parallel}}$ in the exponential factor $\sim \exp(\Delta E_{n,k_{\parallel}}/2k_B T)$, but such an
 enhancement is flattened out as \( T \) goes up to 400 K due to the fact of \( \exp(\Delta E_{n,k} / 2k_B T) \rightarrow 1 \) in this case. Similarly, switching from the \( n = 1 \) ground state to \( n = 2 \) excited state reduces \( \Delta E_{n,k} \), and then pushes down the rate \( T_n(k, T, \xi) \) by three orders of magnitude in figure 3(d). Finally, as displayed in figures 3(e) and (f), it is revealed that the transition rate \( T_n(k, T, \xi) \) becomes largely independent of \( \xi \) within the range of \( \xi \leq \ell_0 \). This feature is attributed to the fact that the void binding radius \( a_d \) is much larger than the quantum-well width \( 2\ell_0 = 2\sqrt{\hbar/m^*\omega_0} \) in this case, and therefore, \( \left| \langle \psi_{n,l=0}(r, z - \xi) | U_{\text{cap}}(r, z) | \phi_{k}(r, z) \rangle \right|^2 \) in equation (36) becomes independent of \( \xi \) as can be verified from equations (37) and (38). However, such \( \xi \) dependence in \( T_n(k, T, \xi) \) will be fully recovered once the condition \( a_d \leq \ell_0 \) or \( |\xi - \ell_0| > a_d \) is satisfied.

We know that the subsystem for conduction electrons only is not a canonical one since the total number of conduction electrons varies with time due to nonzero \( \rho_{\text{cap}}(T, u_0, E^*) \) from equation (48) for captured electrons. In figure 4(a), by including the defect-capture contributions \( \rho_{\text{cap}}(T, u_0, E^*) \), we show the self-consistently calculated chemical potential \( u_0(T) \) as a function of temperature \( T \) for different values of doping density \( n_{\text{dop}} \). In this case, \( u_0(T) \) appears increasing with \( n_{\text{dop}} \) for each given \( T \) but decreasing from positive to negative for fixed \( n_{\text{dop}} \) as \( T \) goes up. Due to the presence of \( \rho_{\text{cap}}(T, u_0, E^*) \) in equation (49), we find from figure 4(b) that the variation \( \delta u_0(T) = u_0(T) - u_0^0(T) \) of the chemical potential, corresponding to a thermal-equilibrium one for \( \rho_{\text{cap}}(T, u_0, E^*) = 0 \), depends on \( T \) in a non-monotonic way and exhibits an initial rolling down followed by a sharp rising around its negative minimum. This unique corner-like feature reveals the fundamental non-canonical role played by \( \rho_{\text{cap}}(T, u_0, E^*) \) for given \( n_{\text{dop}} \) and is attributed to an interplay between the increasing defect-relaxation time \( \tau_{d, \text{rel}}(T, u_0, E^*) \sim 10^{12} \) s and the decreasing defect-capture rate \( \gamma_{\text{cap}}(T, u_0, E^*) \sim 10^{13} \) s\(^{-1} \) as
Figure 4. Temperature dependence of calculated chemical potential \( u_0(T) \) from equation (48) and (49) in (a) and its variation \( \delta u_0(T) = u_0(T) - u_0^{(0)}(T) \) in (b) with \( u_0^{(0)}(T) \) as the chemical potential corresponding to \( \rho_\text{cap}(T, u_0, E^*) = 0 \), along with the defect-relaxation time \( \tau_d^{rel}(T, u_0, E^*) \) from equation (43) in (c) and (d), the defect-capture rate \( \gamma_d^{cap}(T, u_0, E^*) \) from equation (46) in (e) and (f), and the defect-escape rate \( \gamma_d^{esc}(T, u_0, E^*) \) from equation (47) in (g) and (h), for different values of \( n_{\text{dop}} \) and \( E^* \). Here, the vertical scales in panels (b), (d), (g) and (h) are amplified by factors of 10^3 10^4 10^8 10^9, respectively, while the vertical scale in panel (f) is compressed by a factor of 10^{-1}. Moreover, the dashed lines in (a) and (b) indicate the zero scale.

Functions of \( T \), as elucidated by unique physics mechanism presented in equation (48). The increasing \( \tau_d^{rel}(T, u_0, E^*) \) in equation (43) and the decreasing defect-capture rate \( \gamma_d^{cap}(T, u_0, E^*) \) equation (46) as functions of \( T \) are shown in figures 4(c)–(f), respectively. Both thermally-reduced

1/\( \tau_d^{rel}(T u_0 E^*) \) and \( \gamma_d^{cap}(T, u_0, E^*) \) result from decreasing transition rate \( \mathcal{T}_n(k_B T) \) with \( T \). Meanwhile, we find \( \delta u_0(T) \) increases slightly with \( |E^*| \) around the corner. However, \( \tau_d^{rel}(T, u_0, E^*) \) decreases significantly with \( |E^*| \) for high \( T \), in contrast with the slight increase of \( \gamma_d^{cap}(T, u_0, E^*) \) with \( T \). Furthermore, the defect-escape rate \( \gamma_d^{esc}(T, u_0, E^*) (\sim 10^6 \text{ s}^{-1}) \) in figures 4(g) and (h) is also enhanced by increasing \( T \), which comes from the weakening of its exponential factor \( \exp(-\Delta E_{n,k}/k_B T) \) in equation (47) with increasing \( T \), and simultaneously, it increases with growing \( |E^*| \) at high \( T \).
Figure 5. Temperature dependence of calculated capture rate $R_c(k_\parallel, T, E^*)$ of Bloch electrons from equation (12) in (a) and (b), statistically-averaged capture rate $R_c(T, u_0, E^*)$ from equation (18) in (c) and (d), and statistically-averaged energy-relaxation time $\tau_0(T, u_0)$ from equations (22) and (A1) in (e) and (f), as well as current-suppression factor $s_c(T, u_0, E^*) = R_c(T, u_0, E^*)\tau_0(T, u_0)$ in (g) and (h), for various values of $E^*$. Here, the vertical scales in panels (a), (b), (d) and (h) are amplified by factors of $10^3$ $10^4$ $10^4$ $10^3$, respectively.

The average capture rate $\overline{R}_c(T, u_0, E^*)$ from equation (18) for conduction electrons reflects the current suppression and thermal-activation feature for electron transport in quantum wells. By applying the calculated defect transition rate $\overline{T}_d(k_\parallel, T)$ to equation (12), we display in figures 5(a) and (b) the capture rate $R_c(k_\parallel, T, E^*)$ ($\sim 10^{11}$ s$^{-1}$) of Bloch electrons as a function of temperature $T$ for different values of $E^*$. In this case, $R_c(k_\parallel, T, E^*)$ is found decreasing with $T$ but is enhanced by $|E^*|$ at each given $T$. Meanwhile, $\overline{R}_c(k_\parallel, T, E^*)$ increases with $k_\parallel$ because of $\overline{T}_d(k_\parallel, T, \xi)$ as demonstrated in figures 3(c) and (d). Additionally, the statistically-average capture rate $\overline{R}_c(T, u_0, E^*)$ ($\sim 10^{14}$ s$^{-1}$) is shown in figures 5(c) and (d) as a function of $T$ for various values of $E^*$, and it depends on $u_0(T)$ and reduces with increasing $T$. Here, we observe that $\overline{R}_c(T, u_0, E^*)$ becomes much bigger at low $T$ but decreases with $T$ much faster in comparison with $R_c(k_\parallel, T, E^*)$ presented in figures 5(a) and (b). Moreover, the very short statistically-average energy-relaxation time $\tau_0(T, u_0)$ ($\sim 10^{-14}$ s) calculated...
Figure 6. Calculated electron–defect interaction $|\mathcal{U}_d(q_\parallel, T)|^2$ from equation (7) for various values of $E^*$ as a function of $q_\parallel$ at $T = 300$ K and $\xi/\ell_0 = 0.5$ in (a), a function of $T$ with $q_\parallel/k_F = 0.5$ and $\xi/\ell_0 = 0.5$ in (b), as well as a function of $\xi$ at $q_\parallel/k_F = 0.5$ and $T = 300$ K in (c). Here, the vertical scales of $|\mathcal{U}_d(q_\parallel, T)|^2$ in all three panels are compressed by a factor of $10^{-4}$.

Figure 7. 3D plots as functions of $q_\parallel$ and $\omega$ for real (Re) and imaginary (Im) parts of the polarization function $\chi_1^{(0)}(q_\parallel, \omega)$ calculated from equation (2) at $T = 150$ K and $500$ K in (a) and (b), respectively, as well as for Re[$\Gamma(q_\parallel, \omega)$] and Im[$\Gamma(q_\parallel, \omega)$] of defect-vertex corrections obtained from equation (8) at $T = 150$ K with $\kappa_0 = 5$ in (c) and (d) and $\kappa_0 = 2$ in (e) and (f).

from equations (22) and (A1) appears in figures 5(e) and (f) as a function of $T$, which is seen increasing with $T$ and enhanced by $E^*$ for fixed $T$. Furthermore, the dimensionless current-suppression factor $s_c(T, u_0, E^*) = \mathcal{R}_c(T, u_0, E^*) \tau_0(T, u_0)$ from equation (26) ($\sim 1.6$ around $100$ K for more than $60\%$ capturing) in figures 5(g) and (h) is found as a fast decreasing function of $T$ in the low-$T$ regime and increases with $|E^*|$. However, we find a very large current-suppression factor as $T$ becomes much lower than $100$ K. For $T > 150$ K, on the other hand, we see $s_c(T, u_0, E^*) \ll 1$ for a weak-capturing process and it becomes negligible above $300$ K.

The interaction dynamics between electrons and defects can be very well seen from the $T$-dependent effective charge number $Z_{\text{eff}}(T, E^*)$ in $|\mathcal{U}_d(q_\parallel, T)|^2$ from equation (7).
Figure 8. The calculated $\omega$-derivative of imaginary parts of the polarization function $\partial \Im[\tilde{\chi}(q, \omega)]/\partial \omega$ from equations (9), (1) and (2) at $\omega = 0$ as a function of $q_{\parallel}$ with different temperatures $T$ for single ($N = 1$) and triple ($N = 3$) quantum wells are displayed in (a)–(d), respectively, where we assume $\kappa_0 = 2.0$ and 5.0 in (a) and (c) and in (b) and (d). Meanwhile, the obtained inverse of momentum-relaxation times $1/\tau_p$ from equation (35) with $\kappa_0 = 2.0$ and 5.0 as a function of $T$ are presented in (e) and (f) for single and triple quantum wells.
The calculated Hall $\mu_{H}(T, u_{0}, B_{3})$ and longitudinal $\mu_{L}(T, u_{0}, B_{3})$ mobilities from equation (B12) are displayed in (a) and (b) in (c) and (d), respectively, as a function of perpendicular magnetic field $B_{3}$ for different temperatures $T$ with $\kappa_{0} = 2.0, N = 1$ in (a) and (c) and with $\kappa_{0} = 5.0, N = 3$ in (b) and (d). Moreover, $\mu_{H}(T, u_{0}, B_{3})$ and $\mu_{L}(T, u_{0}, B_{3})$ as a function of $T$ are also presented in (e) and (f) for various combinations of $N = 1, 3$ and $\kappa_{0} = 2.0, 5.0$. Here, factors of $10^{4}$ and $10^{5}$ have been introduced in (b) and in (a), (d) and (e).

We have presented the bare polarization function $\chi_{1}^{(0)}(q_{||}, \omega)$ in equation (2), while its defect-vertex correction, as well as its intrawell screening correction, are given in equations (1) and (3), respectively, for single-well ($N = 1$) systems. Meanwhile, we have also included the interwell screening correction in equation (9) for multi-well ($N > 1$) systems. From figure 8(a), for $N = 1$ we first find that $\partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega = \partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega$ at $\omega = 0$ decreases with $q_{||}$ from its resonance peak at $q_{||} = 0$ for each fixed temperature $T$ until approaching zero as $q_{||}/k_{F} \gg 1$. Interwell screening correction also reduces with increasing $T$ at the same time due to occupation of high-energy states. As $\kappa_{0}$ is lifted from 2.0 to 5.0 in figure 8(b), $\partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega$ at $\omega = 0$ is further reduced because of enhanced vertex-correction $\Gamma(q_{||}, \omega)$ and then screening effect $\epsilon(q_{||}, \omega)$ in equation (3), as indicated by equation (1). For $N = 3$ in figures 8(c) and (d), $\partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega$ at $\omega = 0$ increases proportionally in this case compared to the results in figures 8(a) and (b) correspondingly, which stems from the simple fact that $\tilde{\chi}(q_{||}, \omega) \propto N \chi_{1}(q_{||}, \omega)$. Finally, for inverse momentum-relaxation time $1/\tau_{p}$ presented in figures 8(e) and (f) as a function of temperature $T$, we realize that it decreases with $T$ but increases as $\kappa_{0}$ and (d), respectively, as a function of perpendicular magnetic field $B_{3}$ for different temperatures $T$ with $\kappa_{0} = 2.0, N = 1$ in (a) and (c) and with $\kappa_{0} = 5.0, N = 3$ in (b) and (d). Moreover, $\mu_{H}(T, u_{0}, B_{3})$ and $\mu_{L}(T, u_{0}, B_{3})$ as a function of $T$ are also presented in (e) and (f) for various combinations of $N = 1, 3$ and $\kappa_{0} = 2.0, 5.0$. Here, factors of $10^{4}$ and $10^{5}$ have been introduced in (b) and in (a), (d) and (e).

We have presented the bare polarization function $\chi_{1}^{(0)}(q_{||}, \omega)$ in equation (2), while its defect-vertex correction, as well as its intrawell screening correction, are given in equations (1) and (3), respectively, for single-well ($N = 1$) systems. Meanwhile, we have also included the interwell screening correction in equation (9) for multi-well ($N > 1$) systems. From figure 8(a), for $N = 1$ we first find that $\partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega = \partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega$ at $\omega = 0$ decreases with $q_{||}$ from its resonance peak at $q_{||} = 0$ for each fixed temperature $T$ until approaching zero as $q_{||}/k_{F} \gg 1$. Interwell screening correction also reduces with increasing $T$ at the same time due to occupation of high-energy states. As $\kappa_{0}$ is lifted from 2.0 to 5.0 in figure 8(b), $\partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega$ at $\omega = 0$ is further reduced because of enhanced vertex-correction $\Gamma(q_{||}, \omega)$ and then screening effect $\epsilon(q_{||}, \omega)$ in equation (3), as indicated by equation (1). For $N = 3$ in figures 8(c) and (d), $\partial \text{Im}[\chi(q_{||}, \omega)]/\partial \omega$ at $\omega = 0$ increases proportionally in this case compared to the results in figures 8(a) and (b) correspondingly, which stems from the simple fact that $\tilde{\chi}(q_{||}, \omega) \propto N \chi_{1}(q_{||}, \omega)$. Finally, for inverse momentum-relaxation time $1/\tau_{p}$ presented in figures 8(e) and (f) as a function of temperature $T$, we realize that it decreases with $T$ but increases...
with $N$, as found from figures 8(a) and (c). Here, the decrease and increase of $1/\tau_p$ with $T$ and $N$ are caused, separately, by occupation of high-energy states and the relation $\chi(q_1, \omega) \propto N$, as seen clearly from figures 8(a)–(d). Furthermore, $1/\tau_p$ is also strengthened by $\kappa_0$ as expected from the enhanced contribution of $|U_0(q_1)|^2 \propto \kappa_0$ in equation (31) to $1/\tau_p$ in equation (35).

Under a perpendicular magnetic field $B_3$, longitudinal mobility $\mu_L(T, u_0, B_3)$ and Hall mobility $\mu_H(T, u_0, B_3)$ will display different $B_3$ dependence as $\mu_L B_3 \ll 1$ or $\mu_H B_3 \gg 1$. We first present the calculated $\mu_H(T, u_0, B_3)$ as a function of $B_3$ for $N = 1$, $\kappa_0 = 2.0$ in figure 9(a) as well as for $N = 3$, $\kappa_0 = 5.0$ in figure 9(b) with various values of $T$. As $B_3$ increases, $\mu_H(T, u_0, B_3)$ goes up linearly with $\mu^2 B_3$ in figure 9(a) for $\mu_0 B_3 \ll 1$, as shown in equation (B12). Meanwhile, we also find $\mu_H(T, u_0, B_3)$ increasing with $T$ for fixed $B_3$ due to decrease of $1/\tau_p$ as seen from figure 8(e). However, the increase of $\mu_H(T, u_0, B_3)$ with $B_3$ becomes much slower in figure 9(b) for the case with $N = 3$, $\kappa_0 = 5.0$, which can be attributed to the enhanced momentum-relaxation rate $1/\tau_p$ by larger values of $N$ and $\kappa_0$ as can be verified from figure 8(f).

In addition, we also exhibit the calculated $\mu_L(T, u_0, B_3)$ as a function of $B_3$ for $N = 1$, $\kappa_0 = 2.0$ in figure 9(c) and for $N = 3$, $\kappa_0 = 5.0$ in figure 9(d) with various values of $T$. In this case, however, we find $\mu_L(T, u_0, B_3)$ in figures 9(c) and (d) become independent of $B_3$ due to $\mu_0 B_3 \ll 1$ in equation (B12). Moreover, $|\mu_L(T, u_0, B_3)|$ increases with either $N$ or $\kappa_0$, as demonstrated in figure 9(d) and explained by figures 8(e) and 9(f). Finally, both $\mu_L(T, u_0, B_3)$ and $\mu_L(T, u_0, B_3)$ as functions of $T$ are given in figures 9(e) and (f), from which we observe that $\mu_H(T, u_0, B_3)$ and $|\mu_L(T, u_0, B_3)|$ increases with $T$ but decreases with either $N$ or $\kappa_0$, as known from figures 8(e) and 9(f).

7. Summary and remarks

In summary, using many-body theory, we have calculated the modified polarization and dielectric functions of Bloch electrons due to defects in a quantum well. Additionally, we have derived the first two moment equations arising from the semi-classical Boltzmann transport theory. We applied them for investigating self-consistently the dynamical defect interaction effects on the magneto-transport of electrons in a non-canonical subsystem. By using this defect-corrected polarization function, we have obtained analytically both the inverse momentum-relaxation time and the mobility tensor for Bloch electrons. With the use of quantum-statistical theory, on the other hand, we have explored defect capture and charging dynamics based on a parameterized quantum-mechanics model for defects as well as by employing a finite-range probability function. Consequently, we have obtained both the microscopic capture, escape and relaxation rates, as well as the areal density for captured Bloch electrons by defects as functions of temperature, doping density and chosen defect parameters.

Specifically, by employing the energy-balance equation, we have determined the number of occupied energy levels $N^{*}$ and the chemical potential $E^*$ of defects for captured Bloch electrons as a function of temperature $T$ for chosen values of defect binding energy and binding radius. We have also investigated the transition rate $T(k_3, \mu)$ for defect-capturing process as functions of Bloch-electron wave number $k_3$ and $T$. Based on calculated $E^*$ and $T(k_3, \mu)$, we have further explored the defect energy-relaxation rate $\tau_{rel}$, capture rate $\gamma^{cap}$ and escape rate $\gamma^{esc}$, in addition to the self-consistently calculated chemical potential $u_0(T)$ of Bloch electrons in a non-canonical subsystem, as functions of $T$ and doping density $n_{\text{dop}}$. On the other hand, we have further calculated the average Bloch-electron energy-relaxation rate $1/\tau_{rel}(T)$ and momentum-relaxation rate $1/\tau_p(T)$, as well as the Bloch-electron current suppression factor $s_{\text{k}}(T, u_0, E^*)$, as a function of $T$. Finally, we have investigated the perpendicular magnetic-field $B_3$ and temperature $T$ dependence of both Hall $\mu_H(T, B_3)$ and longitudinal $\mu_L(T, B_3)$ mobilities of Bloch electrons in single and triple quantum wells.

Our present theory incorporates a number of different characteristics compared to the well-known BTE. First, we have proposed a parameterized quantum-mechanics-based model for a spherical void by employing a finite-range probability function with independently adjustable binding energy and binding radius. In this way, a new ingredient has been inserted into the nonlocal interaction between defects and conduction electrons. Next, we have introduced an effective charge number to a void for its accommodated electrons, which depends on the surrounding temperature and other bound electrons determined by another proposed energy-balance equation. Consequently, the Coulomb interaction between charged voids and conduction electrons will rely on the external temperature as well as the internal chemical potential of a charged void. Finally, using many-body theory, we have put forward a relationship between the frequency-derivative of the defect-corrected polarization function and the inverse momentum-relaxation time of scattered electrons. Consequently, instead of conventional Boltzmann transport theory, we are able to use this new formalism for exploring defect-limited transport properties of electrons in quantum wells.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Energy-relaxation time

By using the detailed-balance condition, the energy-relaxation time $\tau_{rel}(k_3)$ initially introduced in equation (22) for defects can
where $\sigma_d$ is the defect areal density. The scattering-in rate for electrons in the final $k_f$-state is

$$W_{in}(k_f) = \frac{2\pi\sigma_d}{\hbar A} \int_{q_0} \left| U_0(q_0) \right|^2 \left[ f_{k_f+q_0} \delta(\varepsilon_{k_f} - \varepsilon_{k_f+q_0}) + f_{k_f-q_0} \delta(\varepsilon_{k_f} - \varepsilon_{k_f-q_0}) \right] dq_0,$$

and the scattering-out rate for electrons in the initial $k$-state is

$$W_{out}(k) = \frac{2\pi\sigma_d}{\hbar A} \int_{q_0} \left| U_0(q_0) \right|^2 \left[ f_0(\varepsilon_{k}) \right] \left[ 1 - f_0(\varepsilon_{k}) \right] dq_0.$$

For simplicity, we have introduced the notations, i.e., $f_{k_f} \equiv f_0(\varepsilon_{k_f} - u_0)$. We further assume that electrons are remotely doped, temperature $T$ is low, and areal doped-electron density $\rho_0$ is low. As a result, we can neglect the electron scatterings with ionized impurities, lattice phonons and other electrons, and retain the electron scattering only with charged defects in the system.

For the electron–defect scattering in a quantum well, its interaction introduced in equations (A2) and (A3) takes the form

$$\left| U_0(q_0) \right|^2 = \left( \frac{a_0}{a_d} \right)^2 \left[ \frac{Z_{eff}(T, E^*) e^{\xi_0}}{2\varepsilon_0 e_0} \right] \left( q_{\parallel} + q_{\perp} \right)^2$$

$$\times \int_{-Z_{eff}/2}^{Z_{eff}/2} dz \int_{0}^{\infty} dz' |F_0(z')|^2$$

$$\times \left( e^{-z|z'-\xi|} + e^{-q_{\parallel}|z'+\xi|} \right)$$

$$\times Q_1(q_{\parallel}, q_{\perp} - \xi), \quad \text{(A4)}$$

where $Z_{eff}(T, E^*)$ is the effective charge number of defects, $a_d$ and $a_0 = 5 \text{ Å}$ are the void and point-vacancy binding radii, $e_0$ is the dielectric constant of the host semiconductor, $1/q_s$ is the inverse of a static screening length, $A_1$ is the in-plane correlation length for randomly-distributed defects, the partial form factor $Q_1(q_{\parallel}, \xi)$ is given by equation (C11), and $\rho_0(\xi)$ stands for a linear density distribution of defects.

**Appendix B. Mobility tensor**

From the force-balance equation in equation (23), by using $\tau_{p,-1}^{\ast} = (1/\tau_p)\delta_{ij}$ for simplicity, we get the following two inhomogeneous linear equations for $v_d = \{v_1, v_2, 0\}$

$$(1 + q_{r_1} r_{12} B_3) v_1 - q_{r_1} r_{11} B_3 v_2 = q_{r_1} (r_{11} E_1 + r_{12} E_2)$$

$$(1 - q_{r_2} r_{21} B_3) v_1 + (1 - q_{r_1} r_{12} B_3) v_2 = q_{r_2} (r_{21} E_1 + r_{22} E_2)$$

where we have used the notations $B = \{0, 0, B_3\}$, $E = \{E_1, E_2, 0\}$, and $\tilde{M}^{\ast -1} = \{r_{ij}\}$ for $i, j = 1, 2$. By defining the coefficient matrix $\tilde{C}$ for the above linear equations, i.e.,

$$\tilde{C} = \left[ \begin{array}{c} 1 + q_{r_1} r_{12} B_3 \\ q_{r_2} r_{21} B_3 \\ 1 - q_{r_2} r_{21} B_3 \end{array} \right], \quad \text{(B3)}$$

as well as the source vector $s$, given by

$$s = \left[ q_{r_1} (r_{11} E_1 + r_{12} E_2) \right] q_{r_2} (r_{21} E_1 + r_{22} E_2)$$

we can reduce the above linear equations to a matrix equation

$$\tilde{\Delta} \cdot v_d = s$$

Explicitly, we find the solution $v_d = \{v_1, v_2, 0\}$ for $j = 1, 2$ by

$$v_j = \frac{\text{Det}(\tilde{\Delta}_j)}{\text{Det}(\tilde{C})}$$

where

$$\tilde{\Delta}_1 = \left[ q_{r_1} (r_{11} E_1 + r_{12} E_2) - q_{r_1} r_{11} B_3 q_{r_2} r_{21} B_3 \right]$$

$$\tilde{\Delta}_2 = \left[ q_{r_2} r_{21} B_3 \right]$$

Moreover, by assuming $r_{ij} = 0$ for $i \neq j$, $r_{jj} = 1/m_j^\ast$, and introducing the notation $\mu_j = q_{r_j} m_j^\ast$, we find

$$\tilde{C} = \left[ \begin{array}{c} 1 \\ \mu_2 B_3 \\ 1 \end{array} \right], \quad \text{(B8)}$$

$$\tilde{\Delta}_1 = \left[ \begin{array}{c} \mu_1 E_1 - \mu_1 B_3 \\ \mu_2 E_1 - \mu_1 B_3 \end{array} \right], \quad \text{(B9)}$$

$$\tilde{\Delta}_2 = \left[ \begin{array}{c} \mu_1 E_1 \\ \mu_2 E_1 \end{array} \right]$$

and

$$\text{Det}(\tilde{C}) = 1 + \mu_1 \mu_2 B_3^2.$$
Det\{Δ_1\} = \mu_1E_1 + \mu_1\mu_2B_3E_2,

Det\{Δ_2\} = \mu_2E_2 - \mu_2\mu_1B_1E_1.

From the above results, we finally arrive at

\[ \hat{\mu}(B_3) = \frac{1}{1 + \mu_1\mu_2B_3} \left[ \mu_1 \frac{\mu_1\mu_2B_3}{\mu_2} \right]. \]  

(B11)

If we further assume \( q = -e \), \( m^*_e = m^*_l = m^* \) and \( \tau_1 = \tau_2 = \tau_p \), we obtain 

\[ \text{Det}\{C\} = 1 + \mu_0^2B_3^2, \]

\[ \text{Det}\{Δ_1\} = -\mu_0E_1 + \mu_0^2B_3E_2, \]

and 

\[ \text{Det}\{Δ_2\} = \mu_0E_2 - \mu_0^2B_3E_1, \]

where \( \mu_0 = e\tau_p/m^* \). This gives rise to

\[ \hat{\mu}(B) = \frac{\mu_0}{1 + \mu_0^2B_3^2} \left[ \frac{1}{\mu_0B_3} - \frac{\mu_0}{1} \right]. \]  

(B12)

**Appendix C. Defect effective potential and occupation**

The Schrödinger equation for electrons bounded to a defect can be formally written as [44]

\[ \frac{-\hbar^2}{2m^*} \nabla^2 r \psi_n(r) + [V_L(r) - V_D(r)] \psi_n(r) = E_n \psi_n(r), \]  

(C1)

where \( V_L(r) \) is the full crystal lattice-potential energy, \( V_D(r) \approx V_L(r) - U_D(r) \) represents the deformed lattice-potential energy by a defect, \( U_D(r) \) is the local atomic-potential energy for a point vacancy, \( m^* \) is the effective mass of Bloch electrons, and \( \psi_n(r) \) and \( E_n \) are the eigen-function and eigen-energy of defect-bound electrons, respectively. The accurate calculation of \( V_D(r) \) can be done with first-principles density-functional theory for a point defect [2,4,44].

For simplicity, we assume \( U_D(r) = -Zq/e^2/4\pi\varepsilon_0\epsilon_r r \) for a spherical defect with \( \varepsilon_0 \) approximately as a net charge number and \( \varepsilon_r \) being the dielectric constant of a host material. Moreover, we assume the defect-state energy levels \( E_n = \hbar^2 r^2/2m_0 \) for the principal quantum number \( n = 1, 2, 3, \ldots \), \( E_0 \) for the binding energy, and \( a_0 \) for the void radius, as well as the corresponding wave functions

\[ \psi_{\ell,m}(r) \equiv \psi_{n,\ell,m}(r) = R_{\ell,m}(r) T_{\ell,m}(\cos \theta) \frac{\sin^n \theta}{\sqrt{2\pi}}, \]

\[ R_{\ell,m}(r) = N^{(1)}_{\ell,m} \left( \frac{2r^2}{n} \right) \frac{\Gamma(2\ell+1)}{\Gamma(n+\ell+1)} \frac{\Gamma(n)}{\Gamma(n+\ell+1)}, \]  

(C2)

where \( r \equiv \{r_1, r_2\} \) is a three-dimensional position vector, the angular-momentum quantum number \( \ell = 0, 1, 2, \ldots, n-1 \), the magnetic quantum number \( m = 0, \pm 1, \pm 2, \ldots, \pm \ell \), \( \hbar = \sqrt{\hbar^2 + z^2} \), \( \cos \theta = z/r \), \( r^* = r/a_0 \), and the two normalization factors are given by

\[ N^{(1)}_{\ell,m} = \sqrt{\frac{2}{m_0 a_0}} \frac{1}{(n-\ell-1)!} \frac{1}{2n(n+\ell)!} \]

\[ N^{(2)}_{\ell,m} = \sqrt{\frac{2(\ell+1)}{2(\ell+|m|)!}} \]

Additionally, \( L^{(1)}_m(x) \) in equation (C3) is the generalized Laguerre polynomial, and \( P^\ell_m(x) \) is the associated Legendre polynomial.

Using the obtained bound-electron energy levels \( E_n = -E_0/n^2 \) and wave functions \( \psi_{n,\ell,m}(r) \) in equation (C3), the effective potential energy \( U_{\text{eff}}(r) \) of a charged defect takes the form

\[ U_{\text{eff}}(r) = \frac{2e^2}{4\pi\varepsilon_0\epsilon_r} \sum_{n=1}^\infty f_0(E_n - E^*) \sum_{\ell,m} \int d^3r' \frac{|\psi_{n,\ell,m}(r')|^2}{|r - r'|}, \]  

(C3)

where \( f_0(x) = \left[ 1 + \exp(x/k_BT) \right]^{-1} \) is the Fermi function, \( E^* \in \max\{-E_0, 0\} \) is the Fermi energy for bound electrons inside a defect, and \( T \) is the lattice temperature. If we simply replace \( |\psi_{n,\ell,m}(r')|^2 \) in equation (C3) by a \( \delta \)-function \( \delta(r') \), \( U_{\text{eff}}(r) \) reduces to the well-known Coulomb potential energy \( U_c(r) = \frac{Ze^2}{4\pi\varepsilon_0\epsilon_r r^2} \) with

\[ Z_{\text{eff}}(T, E^*) = \sum_{n=1}^\infty n^2 f_0(E_n - E^*) \]  

(C4)

as an effective charge number, where the assumption of \( k_BT \) much less than the level separation \( \Delta E_n \) is applied in the last step, and both the orbital and spin degeneracies of bound electrons are included.

By introducing a two-dimensional (2D) Fourier transform for a quantum-well system, we have

\[ \frac{1}{|r - r'|} = \frac{2\pi}{A} \sum_{q_i} \exp[iq_i \cdot (r_1 - r_1')] e^{-q_i [z' - z]} q_i, \]  

(C5)

where \( A \) stands for the area of the quantum well. Then, from equation (C5) we get the 2D Fourier transformed \( U_{\text{eff}}(q_i, z) \), given by

\[ U_{\text{eff}}(q_i, z) = \int d^2r_1 U_{\text{eff}}(r_1, z) \exp(-iq_i \cdot r_1) \]

\[ = \frac{e^2}{\hbar^2 a_0} \sum_{n=1}^\infty f_0(E_n - E^*) \times \int d^2r' \ e^{-q_i [z' - z]} Q_n(q_i, z'), \]  

(C6)

where the partial form factor \( Q_n(q_i, z') \) is defined as

\[ Q_n(q_i, z') = \int d^2r'_1 \exp(-iq_i \cdot r'_1) \sum_{\ell,m} |\psi_{n,\ell,m}(r'_1, z')|^2. \]  

(C7)
By approximating
\[ |\psi_{n,l}(r, z)|^2 \approx \frac{1}{\pi} \left( \frac{1}{a_d} \right)^3 \exp \left[ -\left( \frac{2}{a_d} \right) \left( r^2 + z^2 \right)^{1/2} \right] \]
for the lowest \( n = 1 \) eigenstate, we arrive at an explicit expression
\[
U_{\text{eff}}(q_i, z) \approx \frac{Z_{\text{eff}}(T, E^*)}{2\epsilon_0(\epsilon_i + q_d)} \int_{-\infty}^{\infty} dz' e^{-q_i|z-z'|} e^{-\eta_0^2z'^2/4} \times Q_1(q_i, z'),
\]
where
\[
Q_1(q_i, z) = 2 \left( \frac{1}{a_d} \right)^3 \int_0^{\infty} dr |J_0(q_i r)| e^{-q_i r} \sqrt{r + z^2},
\]
\[
J_0(x) \text{ is the first-kind Bessel function of order zero, and its contribution becomes negligible for either } r/A_d \gg 1 \text{ or } |z|/a_d \gg 1.
\]

Physically, we still need to determine the value of \( E^* \) for thermal-equilibrium distribution of bound electrons accommodated by a defect. Considering the increased Coulomb repulsion by accommodating more and more electrons with a defect, we first introduce the following quantum-mechanical energy-balance equation, i.e.,
\[
e^2 \sum_{l=0}^{\infty} \sum_{n'=1}^{n} \frac{2\ell + 1}{|R_{n', n+1} - \bar{R}_{l,l}|} - \frac{n_0^2}{2}\left[ \frac{E_d}{(n + 1)^2} \right] = 0,
\]
where \( n'(E_d, a_d) \in \{1, 2, 3, \ldots \} \), which represents the index of the topmost occupied energy level of the defect, is the root of equation (C12), \( \hbar \omega_0/2 \) is the lowest subband edge, and the quantum-mechanically average orbital radii of bound electrons are
\[
\bar{R}_{nl} = \int_0^{\infty} |R_{nl}(r)|^2 r^2 dr = s^2 a_d \left[ 1 + \frac{1}{2} \left( 1 - \frac{\ell(\ell + 1)}{s^2} \right) \right],
\]
\[
\bar{R}_{n', n+1} = \frac{n_0^2}{n + 1} \sum_{l=0}^{\infty} \bar{R}_{n'+1, l}.
\]

By using this obtained index \( n'(E_d, a_d) \), the total number \( N'(E_d, a_d) \) for bound electrons is calculated as \( N'(E_d, a_d) = 2\sum_{n=1}^{n'} s^2 \) including spin degeneracy. Next, for a given value \( N'(E_d, a_d) \) resulting from the root of equation (C12), we further put forward the following particle-number conservation equation to include the thermal effect at temperature \( T \), yielding
\[
2 \sum_{n=1}^{\infty} \frac{n^2}{1 + \exp((E_n - E^*)/k_BT)} - N'(E_d, a_d) = 0,
\]
where the temperature-dependent \( E'(T, N') \) is the root of equation (C15) and represents the 'chemical potential' for bound electrons in a defect.

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