1. Introduction

Point defects are ubiquitous in real crystals. Imperfections, vacancies and interstitials, can alter major physical properties of solids such as the phonon spectrum, as well as optical and electrical properties to some extent [1].

Defects in semiconductors such as Si, Ge and compound semiconductors such as GaAs in general dissolve on lattice sites creating shallow point-like acceptors or donors, which make them suitable for electronic and spintronic device applications [2, 3]. In general ionized impurities affect the carrier dynamics in bulk semiconductors at high doping concentrations or at low temperatures, see [4, 5].

Different theoretical approaches have been proposed to tackle the problem of interactions between point-like ionized impurities and electrons in solids. The standard tools are: the Green’s function formalism [6], density functional theory (DFT) [7–9] and first order time-dependent perturbation theory of quantum mechanics [10]. Assuming that the impurities, which are randomly distributed centers in bulk semiconductors, cause small perturbations, and neglecting exchange and correlation effects, one can apply the linear response theory (LRT) in random phase approximation (RPA). Then in the limit of small wave vector transfer, i.e. when a linearized Thomas–Fermi approximation (LTFA) holds, a screened Coulomb potential of Yukawa form is sufficient to accurately account for electron-impurity (e-i) interaction. By means of this impurity potential, the scattering probability for a single (incoherent) electron-impurity collision, is computed via the Fermi golden rule (FGR). This important result is often referred to as Brooks-Herring (B-H) approach [4, 11, 12].

Note that this simple model neglects the perturbing effects of the impurities on the carrier energy levels and wave functions [13]. However, despite its simplicity, it is able of giving
quantitatively accurate carrier mobilities for most of cases of interest, and is routinely employed in ensemble Monte Carlo (EMC) simulations of carrier transport [14, 15].

The Brooks-Herring model has the amenable property to make the electron-impurity scattering problem tractable [16]. However, Fermi’s golden rule entails the first Born approximation (B1), whose validity becomes questionable in the low energy limit [17]. As a consequence, it was found that in general, the B-H approach overestimates the electron-impurity interactions at low energies, see [18]. In the following we make no attempt to investigate the limits of the Born approximation, which have been addressed in many other papers [4, 13, 19, 20], by assuming that the electron-impurity potential is of Yukawa form. As the B-H model rests on the combination of two basic approximations, i.e. B1 and RPA, different authors have tried to improve it by bypassing these central approximations. One possible attempt to overcome B1, needs to include quantum corrections such as the second (B2) and third Born approximations, coherent scattering from pairs of distinct impurity centers, and dressing effects of impurities on the carriers’ energy spectrum and wave functions [13]. In this case, the carrier and impurities continue to interact via a Yukawa potential, i.e. the impurity potential is still evaluated at RPA level. In general, it is found that for for a n-type GaAs, these corrections become questionable for concentrations smaller than $10^{18}$ cm$^{-3}$ [4, 13, 21]. The alternative approach to bypass the B1, can be pursued by including the contribution to the scattering probability from all the terms of the Born series via the partial-wave analysis [22]. Very recently, this was also achieved through the phase variable method (VPM), which computes the scattering phase shifts accurately [23].

On the other hand, improving over the RPA, by including exchange and correlations effects, is also viable [24]. In semiconductor physics literature, accounting for these many-body effects, is often referred to as Takimoto screening [18, 25]. Note that introducing these many-body corrections to the simple RPA, the impurity potential typically takes the form of an exponent cosine screened Coulomb potential. The latter is routinely employed in plasma physics, see [26]. Instead, in the bulk semiconductor physics, this potential is scarcely used, as it can model the e-i interactions meaningfully only for dopant concentrations much smaller than $10^{17}$ cm$^{-3}$ [18].

In this paper, we investigate how the Brooks-Herring model invalidates the LTFA through the electron-impurity scattering kinematics, in the degenerate regime, i.e. for temperatures $T$ much smaller than Fermi temperature $T_F$, in n-type semiconductors. To this end, we consider the carrier dynamics in bulk n-type GaAs semiconductor whose material parameters (doping, temperatures) are chosen to ensure that the basic conditions on which the Brooks-Herring model rests, are satisfied.

To address this inconsistency, we study the wave vector, or equivalently the momentum, transfer due to the e-i intra-valley elastic collisions within the linear response theory for an electron liquid. The polar scattering angles, consistent with the B-H model, are stochastically generated by means of a particular EMC algorithm, for a large number of scattering events [14, 15]. This algorithm allows us to obtain the wave vector transfer distribution for the material parameters under scrutiny.

Our findings show that the average wave vector transfer is $\bar{q} \sim 0.7k_F$, where $k_F$ is the Fermi wave vector. This result manifestly invalidates the LTFA, which hold only for $q \sim 0$ (or equivalently $q \ll k_F$) [1, 24]. Therefore, the B-H approach proves unable to prevent large wave vector transfer. On the other hand, we previously found that in general this does not occur when the carrier dynamics is studied in a nondegenerate regime [23]. In the latter case, the self-consistency between the LTFA and B-H model is correctly achieved.

Additionally, as the linear TF screening, does not distinguish between attractive and repulsive Coulomb interaction, we address the effects of the inverse screening length, computed up to the second Born approximation, on the momentum transfer. It could be believed that that this screening modification, which rests on the Friedel sum rule (FSR), could prevent large momentum transfer, previously observed in the electron-impurity scattering processes. However, our findings prove that indeed it is not always ($\bar{q} \sim 0.8k_F$).

Finally, our analysis of the case $q$-dependence of the B1 electron-impurity differential cross-sections, shows that small discrepancies, of about 1%, arise between the scattering probabilities due to the impurity potentials in LTFA, i.e. of Yukawa form, and in RPA respectively, for the most relevant $q$ values.

This paper is organized as follows. In section 2 we recall the main results about the linear response theory for the electron liquid, including the derivation of the LTFA inverse screening length at finite temperature, and the derivation of the electron-impurity scattering rate in B1. In section 3 we study the wave vector transfer distribution in n-type GaAs. Moreover, we show that all the basic criteria for the validity of the B-H model, are completely satisfied for the chosen material parameters. In section 4 we present the effects of the B2 inverse screening on the momentum transfer. We also include all the necessary formalism to make the screening parameter (impurity) charge-dependent. Finally, in section 5 the behavior of the e-i differential cross-sections against the wave vector transfer is illustrated for the material parameters under scrutiny. We also discuss the physical significance attached to the wave vector transfer, which mainly motivated this work.

2. Electron-test charge interaction in linear response theory at RPA level

The model of impurity screening we employ idealizes the actual situation of a realistic positive ion embedded in a weakly interacting electron gas in a paramagnetic state. In fact an impurity, like proton in the Hydrogen atom, is a source of a strong perturbation to the electron gas surrounding it, giving rise to non-linearity effects stronger in the vicinity of the impurity where the electron density becomes large enough to make the LRT approach questionable [27, 28]. In the following we will limit ourselves to the linear response theory. In order to estimate the screened electron-impurity interaction at RPA level, we need the finite temperature density-density response function $\chi_{nn}(q, \omega, T)$, where $q, \omega$ are the wave vector and the
frequency respectively, for a homogeneous three-dimensional non-interacting electron gas in a paramagnetic state. The real and imaginary parts of $\chi_{nm}$ read [24, 29]

$$\frac{\text{Re} \chi_{nm}(q, \omega, T)}{N(0)} = -\int_0^{\infty} dx F(x, T) \frac{\omega}{2q} \left( \ln \left| \frac{x - v_-}{x + v_+} \right| - \ln \left| \frac{x - v_+}{x + v_-} \right| \right),$$

and

$$\frac{\text{Im} \chi_{nm}(q, \omega, T)}{N(0)} = -\frac{\pi}{2} \left( \frac{\omega}{q v_F} + \frac{k_B T}{\hbar q v_F} \ln \frac{1 + e^{\beta [\varepsilon - \mu - \varepsilon_F]}}{1 + e^{\beta [\varepsilon - \mu + \varepsilon_F]}} \right),$$

respectively. In equations (1) and (2) we have introduced the following dimensionless variables $\bar{q} = q/k_F$, and $\bar{v}_\pm = \omega/v_F \pm q/2k_F$ where $k_F$ and $v_F = h k_F/m^*$ are the Fermi wave vector and Fermi velocity respectively, $m^*$ being the carriers’ effective mass. The symbol $N(0) \equiv m k_F^2/\pi^2 \hbar^2$ denotes the total density of states per unit volume at the Fermi energy for an electron gas in a paramagnetic state, $\hbar$ being the reduced Planck constant.

In equation (1) the function $F(x, T)$ is given by

$$F(x, T) = \frac{x}{e^{\beta \varepsilon_F} + 1},$$

where $\varepsilon_F, \mu$ are the Fermi energy and the electronic chemical potential respectively. In equation (2) we define $\beta \equiv 1/k_B T$, $k_B$ being the Boltzmann constant.

The presence of impurities would modify $\chi_{nm}$, however we shall be interested only in the static response, and hence this effect can be ignored [24, 30]. The next step is to include the response of an interacting electron liquid through the dynamical RPA dielectric function $\epsilon^{\text{RPA}}(q, \omega, T)$

$$\epsilon^{\text{RPA}}(q, \omega, T) = 1 - v_q \chi_{nm}(q, \omega, T),$$

where $e$ and $Ze$ are the magnitudes of the elementary charge and the impurity charge respectively, and $v_q = -4\pi Z e^2/q^2$ is the Fourier transform of the bare Coulomb potential. Thus the electron-impurity test charge screened interaction at RPA level is

$$V^{\text{TF}}_{\text{ie}}(q, \omega) = \frac{v_q}{\epsilon^{\text{RPA}}(q, \omega, T)}.$$  

For so far the results are quite general, indeed the nonparabolicity and other band-structure effects are expected to give corrections of second order [31], however the impurity potential of the B-H model rests on two more crucial assumptions. First, it considers only static perturbations to the electron system. Second, it assumes that these perturbations occur only in the long wavelength limit, i.e. $q \ll k_F$. The latter provides the Thomas–Fermi approximation for the electron-impurity interaction potential, and shapes the impurity potential into a potential of Yukawa form.

As we shall consider elastic scattering between impurities and electrons, the adiabatic linear response for density fluctuations at finite $q$ in the low-frequency limit, can be obtained by setting $\omega = 0$ in equation (4). Finally, it is possible to expand the dynamic dielectric function (the imaginary part vanishes for $\omega \to 0$, and hence $\text{Re} \epsilon^{\text{RPA}} = \epsilon^{\text{RPA}}$), as the following series [31]

$$\epsilon^{\text{RPA}}(q, 0, T) = 1 + q_0^2 \left[ 1 - \frac{1}{6} \left( \frac{q^2 h^2}{2m^* k_B T} \right) \mathcal{F}_{-3/2} - \frac{1}{60} \left( \frac{q^2 h^2}{2m^* k_B T} \right) \mathcal{F}_{-5/2} \mathcal{F}_{-1/2} - \cdots \right],$$

where $\mathcal{F}_j$ denotes Fermi integral of order $j$ [32], and $q_0$, the finite temperature LTFA inverse screening length at temperature $T$, reads

$$q_0^2 \equiv \frac{4\pi n_e e^2}{k_B T} \mathcal{F}_{-2/3}(\eta) \mathcal{F}_{-1/2}(\eta).$$

Taking the Fourier transform of equation (5), one obtains the Yukawa potential, i.e. $V^{\text{TF}}_{\text{ie}}(r) = -(Ze^2/e) e^{-q_0 r}$ denoting the interparticle distance. The Hartree potential given by equation (9) is a direct consequence of Thomas–Fermi theory [33, 34]. Here we must recall that Thomas–Fermi theory, one of the simplest density functional theories [35], is indeed a very crude approximation. In fact the dielectric function $\epsilon^{\text{RPA}}$ is singular at $k = 2k_F$, giving rise to the long-range oscillations of electronic density at large distances from the impurity center (Friedel oscillations) [24], while the Thomas–Fermi theory cannot explain this phenomenon, because it simply models the electron-impurity interaction as a monotonically decreasing potential.

Next, we derive the electron-impurity scattering rate employed in the Brooks-Herring model which rests on the interaction potential given by equation (9), and on single-site collisions.

In practical calculations, it is customary to handle the scattering between a carrier of Bloch wave vector $k$ and a point-like impurity as a perturbation via Fermi’s golden rule.

The transition rate $w_n$ for a general impurity potential $V_{\text{ie}}(r)$, reads

$$w_n = \frac{2}{\hbar} |\langle k' | V_{\text{ie}}(r) | k \rangle|^2 \delta(E' - E),$$

where $k$, $E$ and $k'$, $E'$ denote the carrier’s wave vectors and energies before and after a collision respectively. Assuming that the electron-impurity scattering is elastic, the wave vector
transfer is \( q = k - k' \) with a scattering angle \( \theta \in [0, \pi] \), see the cartoon in figure 1(top right). Note that in general, the conservation of crystal momentum requires that \( k - k' = \mathbf{q} - \mathbf{G} \) where \( \mathbf{G} \) is a reciprocal wave vector. In GaAs for intravalley collisions, there are no umklapp processes, thus in our case \( \mathbf{G} = 0 \). Therefore the wave vectors \( \mathbf{k'} \) form an Ewald sphere, and the wave vector transfer magnitude \( q \) due to a collisional event is

\[
q^2 = 4 k^2 \sin^2 \left( \frac{\theta}{2} \right).
\]

Clearly, the matrix element of equation (10) is proportional to the \( q \)-component Fourier transform of potential, i.e. \( \propto V_{\text{ei}}(q) \). This is why the Fermi’s golden rule entails the first Born approximation [36]. If we assume that the linear Thomas–Fermi screening holds, that is \( q \to 0 \), then \( V_{\text{ei}}(q) = V_{\text{ei}}^0(q) \), see equation (9). In the latter case, if \( n_i \) denotes the doping concentration, inserting equation (9) in (10), one gets [37]

\[
w_{\text{ei}} = \frac{2 \pi n_i (4 \pi Z e^2)^2 e^4}{\hbar V (q^2 + q_0^2)^2} G_{\text{F}}(E' - E),
\]

where \( V \) is the volume of the solid, and the overlap integral \( G_{\text{F}} \) for transitions between band of index \( n_i' \), \( n \) reads [38]

\[
G(k', k) = \int_{V_c} u_{n_i'}^*(k')u_n(k) \, d\mathbf{r}.
\]

\( V_c \) being the unit cell volume. The symbol \( u_n \) denotes the modulating periodic part of the Bloch functions. Hence, once the semiconductor band-structure is known, the electron–impurity scattering rate, and the wave vector transfer distribution can be derived analytically through equation (12), see the relevant discussion in section 3.

Note that in this derivation we limited ourselves to a weak-scattering regime which ensures that Fermi golden’s rule does not need a modification for including the collisional broadening [39].

3. Wave vector transfer: inverse screening length computed in B1

In this paper we perform sample calculations for a \( n \)-type GaAs. We consider carrier dynamics at the bottom of the central \( \Gamma \) valley in GaAs. Despite this fact, our analysis is certainly quite general and holds for any bulk semiconductor insofar as the carriers can be considering roaming in an ideal spherical conduction band. Hence in the effective-mass approximation Bloch electrons have a scalar effective mass \( m^* \), and the density of states (DOS) can be computed analytically through the parabolic energy dispersion \( E = h^2 k^2 / 2m^* \). The overlap integral \( G_{\text{F}} \) is shown to be unity for the intravalley transitions \( (n' = n) \) in a spherical CB [37]. Moreover without loss of generality, we shall consider only the case of univalent impurities (\( Z = 1 \)).

In the following we study wave vector transfer distribution for a doped GaAs with these band-structure parameters: \( \varepsilon = 12.9 \varepsilon_0, m^* = 0.067 m_e, \varepsilon_0, m_e \) being the vacuum permittivity and the electron bare mass respectively [40]. The doping concentration is \( n_i = 5 \times 10^{17} \text{ cm}^{-3} \), and we shall assume that the electron density \( n_e = n_i \) [5] which, ignoring the crystal lattice structure, corresponds to a homogeneous electron gas (jellium model) at \( T_F \approx 398 \text{ K} \) with Wigner–Seitz radius \( r_s = 0.7 (1/n_e) \approx (4\pi/3) (r_a^0)^3 \), \( r_a^0 \) being the effective Bohr radius. The latter condition guarantees that RPA holds.

Furthermore for this choice of intermediate doping density (smaller than \( \approx 10^{18} \text{ cm}^{-3} \)), one can safely ignore the possibility of multiple scattering events during the carrier dynamics [12] as well as the risk of impurity potential overlapping, and thus possible violations of the FSR [41]. The Meyer and Bartoli’s criterion [42], see (16) and the relative results, seems to suggest that we chose the right material dopant concentration.

We consider e-i scattering events for the range of temperatures \( T = 32–77 \text{ K} \) where carrier dynamics is expected to be degenerate \( (T \ll T_F) \). The degeneracy of the carrier distribution for this doping concentration at \( T = 77 \text{ K} \) is also confirmed by experiments of how carrier heating affects the Burstein shift [43]. It was found that one needs to apply electric fields of strength 200–900V cm\(^{-1}\) to observe a distinct non-Fermi behavior. Then it seems reasonable to assume in good approximation that carriers scatter off impurities as plane waves of Fermi wave vector \( \mathbf{k}_F \) \( (E_F \approx 34 \text{ meV}) \) [44] whose magnitude is \( k_F = (3\pi^2 n_i)^{1/3} \) [30].

The EMC, a numerical method routinely employed for solving Boltzmann transport equation in semiconductors, provides a specific algorithm to stochastically generate the carrier-impurity collisional angles \( \theta_i \) within B-H model, which reads [15]

\[
\cos \theta_i = 1 - \frac{2 (1 - r)}{1 + 4 \gamma r}
\]

(14)
where \( r \) is a uniform random number between 0 and 1 and \( \gamma = E_F/E(\Xi \equiv h^2q_0^2/2m^*) \). Note that this algorithm is derived from equation (12), and thus requires that the band-structure be spherical (effective-mass approximation). Furthermore, it corresponds to a normalized probability density.

The validity criterion of B1 for the Brooks-Herring model requires [4] that

\[
4\gamma \gg 1, \tag{15}
\]

which certainly holds in our case \( (\gamma \approx 2) \). To ascertain that the inequality equation (15) gives a reasonable result, we also computed the exact scattering phase shifts \( \delta_l \) for angular momentum numbers \( l = 0, 1 \), which arise from solving the Schrödinger radial equation in the presence of the impurity potential \( V_{\text{eff}} \), by means of the VPM [23, 45, 46]. We found that their values (in radians) are \( \delta_0 \approx 0.5, \delta_1 \approx 0.2 \), thereby confirming that B1 is a good approximation, being all the phase shifts much smaller than \( \pi/2 \) [23, 47, 48].

For the material parameters under scrutiny, the multi-impurity scattering to electron-impurity scattering, can be also excluded. In fact, the criterion for which the single-ion site picture is formally valid, needs that the dimensionless parameter \( d \), which gives the average number of impurities contained in a sphere of radius \( 1/q_0 \), satisfies the following inequality [42]:

\[
d \lesssim \frac{8}{(1 + 64b^{-3/2})^2}, \tag{16}
\]

where \( b = 4\gamma \). In our case, we found that \( d \approx 0.4 \) while the right-hand side of equation (16) is approximately 2. So, the assumption of independent scattering is certainly satisfied.

In the following we generated \( 10^7 \) e-i collisional events by means of equation (14), for the temperatures of interest \((T = 32 – 77 \text{ K}) \). Note that in EMC simulations the number of collisions is usually larger, however this makes a negligible difference for present analysis. In figure 1 we plot the (normalized) histogram of wave vector transfer due to electron-impurity scattering for \( T = 32 \text{ K} \). In general, partial waves of different angular momentum \( l \) might affect this distribution through their quantum interference. Only performing the events have large scattering angles with \( q \). For the materials under scrutiny, the multipoles s-wave \((l = 0, 1) \), see [5]. Moreover from scattering theory we expect that the partial wave \( l = 1 \) contributes to the angular distribution for energies smaller than those significant for its contribution to the total cross-section [49].

The distribution plotted in figure 1 shows that the maximum of distribution occurs for \( q_{\text{max}} \approx 0.4k_F \) and the wave vector transfer mean value is \( \bar{q} = 0.72k_F \). Additionally, about 10% of the events have large scattering angles with \( \theta \approx \pi/2 \). These results clearly contradict the crucial assumption \( q \ll k_F \) for validity of the Thomas–Fermi approximation, and therefore invalidate the screened Coulomb interaction given by equation (9). We also see that the \( q^2 \) term in the denominator of equation (12) is not sufficient to prevent large \( q \) values. On the other hand, the study of carrier dynamics in a nondegenerate regime clearly showed that in general the wave vector transfer \( q \) during the collisions is negligible [50]. Similar results (not shown) are obtained for all the temperatures of interest.

4. Wave vector transfer: inverse screening length computed in B2

Next, we consider a completely different, but equivalent, approach, which relates the Thomas–Fermi linear screening theory to the nonrelativistic scattering theory on the basis of charge neutrality provided by FSR. This will allow us to accurately compute the inverse screening length in the second Born approximation. The main physical reason to do so, is that the first Born approximation does not distinguish between attractive and repulsive interaction potential. Here, we need to stress that in the following we are not going to compute the scattering rate beyond the first Born approximation, i.e. the Fermi’s golden rule still holds, but the inverse screening length will be ‘optimized’ to the second order in the Born series.

The FSR [51, 52] is a statement for the complete screening of the charge impurity by the surrounding electron gas. For \( n \)-type semiconductors with one parabolic band, FSR reads [53]

\[
\frac{2}{\pi} \sum_{l=0}^{\infty} (l+1) \int_0^\infty f(E) \frac{d\delta_l(E)}{dE} dE = Z, \tag{17}
\]

where \( f \) is the Fermi–Dirac distribution, and \( E \) is the carrier’s collisional energy. Given a general impurity potential \( V_{\text{ei}} \), the phase shifts can be computed in B1 by means of this formula [36]

\[
\delta_{B1}(\eta) = -k_F A_l \tag{18}
\]

with

\[
A_l = \int_0^\infty J_l(k_Fr) U(r) r^2 dr, \tag{19}
\]

where in equation (19) \( J_l \) denote the spherical Bessel functions and we have introduced the reduced potential \( U \equiv (2m^*)V_{\text{ei}}/\hbar^2 \). When \( B1 \) holds, then the \( \delta_l \) are small, and hence \((\tan \delta_l)_{B1} \approx \delta_l \approx \delta_l_{B1} \). In the latter case, if we insert \( \delta_l_{B1} \) into equation (17), we get the following mathematical constraint on the impurity potential [4]

\[
\frac{1}{\sqrt{\pi}b^2} \left( \frac{2m^*}{\hbar^2} \right)^{1/2} \mathcal{F}_{-1/2}(\eta) \int_0^\infty U(r) r^2 dr = Z. \tag{20}
\]

Now, let us assume that the impurity potential takes a Yukawa form, with unknown screening parameter \( q^* \) i.e.

\[
V_{\text{ei}}(r) = -(Z\pi^2/r) e^{-q^* r}, \tag{21}
\]

then, inserting equation (21) into equation (20), one finds that \( q^* \approx \delta_l_{B1} \approx \delta_l \), see equation (7). This is really a remarkable result. Therefore, the inverse screening length can be obtained self-consistently requiring that the phase shifts obey the FSR. The previous procedure suggests how to compute the inverse screening length \( \delta_l_{B2} \) in second Born approximation for a potential of Yukawa form.
The agreement with the Born series through second order, can be achieved by computing \( \zeta_2 = (\tan \delta)_{B1} + (\tan \delta)_{B2} \) where the second addend defines the phase shifts in B2, see [36], for its definition.

In order to avoid the calculation of the two terms separately, i.e. \((\tan \delta)_{B1}\) and \((\tan \delta)_{B2}\), a not easy task due to the rapidly oscillating integrand for a potential of Yukawa form, one can resort to the Schwinger variational principle for the phase shifts. Indeed, by means of the Schwinger variational principle \( \zeta_2 \) is given by [36, 54]

\[
\tan \zeta_2 = -k_F A_1 (1 - B_1 / A_1),
\]

where

\[
B_1 = \int_0^\infty dr \int_0^\infty dr' j_i (k_F r) U (r) G_i (r, r') \times U (r') j_i (k_F r') r^2 r'^2.
\]

In equation (23) we have defined the following function \( G_i (r, r') = k_i (k r_\perp) \eta_i (k r_\perp) \) where \( \eta_i \) are the spherical Neumann functions, and \( r < = \min\{r, r'\} \) and \( r_\perp = \max\{r, r'\} \). In the limit of low temperatures, it is possible to approximately compute \( \zeta_2 \) [54], and hence by means of equations (17) and (21), one can obtain \( q^* \equiv q_{0,B2} \) in a simple closed form

\[
q_{0,B2} = \frac{q_0^2}{s + s^2 + q_0^2},
\]

where \( s \equiv m^* Z e^2 / 8 \pi e \hbar^2 \). Note that now \( q_{0,B2} \) depends upon the impurity charge sign through \( s \), making the sign of \( Z \) discernible. Moreover, we found that for \( Z = 1 \), \( q_{0,B2} > q_0 \). So, the donor impurity potential range becomes shorter due to the B2 approximation.

The average \( q_{B2} \) can be computed again via equation (14) by setting \( \bar{E} = h^2 q_{0,B2}^2 / 2 m^* \). The effects on the average wave vector transfer \( \bar{q} \) due to \( q_{0,B2} \) (diamonds) along with those of \( q_0 \) (circles) are illustrated in figure 2 for the same number of collisions (10^7 events). Note that according to [5] we expect that the B2 becomes important for much lower carrier energies than \( E_F \), that is, when the scattering probability, given by equation (12), becomes weakly dependent on the angle \( \theta \) [5].

In figure 2, the curves show that these averages are nearly constant: \( q_{0,B1} \simeq 0.7 \) and \( q_{0,B2} \simeq 0.8 \) in \( k_F \) units and their variations are about 1%. But the results are even worse for B2, and are a direct consequence of the larger screening lengths due to the phase shifts computed in B2 [5]. These results confirm again that the obtained wave vector transfer distribution is inconsistent with a LTFA.

5. Analysis of differential cross-sections in Born approximation and concluding remarks

From the Fermi golden’s rule is straightforward to derive the differential cross-section \( \sigma^1 (\theta) \) in B1 for a parabolic CB. Given a general potential \( V_\alpha \) one finds [55]

\[
\sigma^{1}_{\alpha} (\theta) = \left( \frac{m^*}{2 \pi \hbar^2} \right)^2 |V_\alpha (q)|^2,
\]

where the \( \theta \)-dependence is implicitly given by equation (11). Hence, by assuming that the carrier’s dynamics occur at the bottom of conduction band, we can define the following quantity \( R = \sigma^{TF}_{\alpha} / \sigma^{RPA}_{\alpha} \) where \( \sigma^{TF}_{\alpha} \) and \( \sigma^{RPA}_{\alpha} \) are the differential cross-sections computed in B1, using the impurity screened potential given by equations (9) and (5) respectively.

In figure 3 we plot \( R \) values for some relevant wave vector transfer, in particular \( q_{\max} \) and \( \bar{q} \) and for temperatures \( T = 32, 52, 77 \) K. Note that, as discussed before, the \( q \) value interval of figure 3 is where the TF approximation completely fails. We observe that the cross-sections differ by less than 1% or \( \sim 1\% \) in the case of \( T = 52 \) K for the majority of collisions, i.e. those for which \( q = q_{\max} = 0.4 k_F \). For larger values of \( q \) the discrepancy increases monotonically, and for \( q \rightarrow 2 k_F \) (not shown) we found that the Brook-Herring model underestimates the scattering probability by roughly 10%. From this analysis we conclude that the B-H model underestimates the scattering...
probabilities when they are compared with those obtained from the exact, at RPA level, impurity potential. However, by virtue of the small discrepancies at the relevant $q$ values, the B-H model still proves useful for practical applications such as EMC.

Sanborn et al [41] argued that strong violations of FSR (equation (17)) may cause a breakdown of the linear response approximation. They stated that these violations occur, whenever the potential $V_{si}$ is strong enough to form its first bound state. This would mean that the first Born approximation does not longer hold. In section 3 we showed that the B1 is valid, thus ensuring that the LRT is certainly applicable to our case.

The physical significance of the momentum transfer can be easily understood from the quantum field theory, which describes the interaction of the electrons with a charge distribution via the exchange of one, or more photons [56]. From this point of view, a large momentum transfer means that the charge distribution has a certain spatial extent. Our findings of sections 3 and 4 seem to suggest that the carriers see the impurities as having some spatial extent for most of the collisional events, while the basic starting assumption of the theory, see section 2, is that the impurities are point-like charges. Moreover, in real semiconductors, the disorder would break the translational symmetry locally. On the other hand, the translational symmetry underpins the linear response theory and the scattering theory, we presented in section 2, and hence the B-H model. Thus, one may wonder how to include the effects of disorder in the present formalism, and how this may affect the wave vector transfer distribution.

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