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Quantum and classical scattering times due to charged dislocations in an impure electron gas

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We derive the ratio of transport and single-particle relaxation times in three- and two-dimensional electron gases due to scattering from charged dislocations in semiconductors. The results are compared to the respective relaxation times due to randomly placed charged impurities. We find that the ratio is larger than the case of ionized impurity scattering in both three- and two-dimensional electron transport.

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In their work on the transport properties of impure metallic systems, Das Sarma and Stern[1] show the difference between two characteristic relaxation times for the case of scattering from randomly located charged impurities. They make a clear distinction between the transport scattering time τ_t and the quantum scattering time (or the single-particle relaxation time) τ_q.

Whilst the quantum scattering time is a measure of the time spent by a carrier in a particular momentum eigenstate state $|\mathbf{k}\rangle$ in the presence of a perturbing (or scattering) potential, the transport scattering time is the measure of the time spent in *moving along the applied field*;[2] the lifetime thus gets weighted by an angular contribution factor $(1-\cos\theta)$ that enhances the small-angle scattering contribution to the relaxation rate over large-angle scattering. Thus, the scattering rate is defined to be

$$\frac{1}{\tau}=\sum_{k'} S(\mathbf{k}',\mathbf{k})f(\theta), \tag{1}$$

where $f(\theta)=1$ and $(1-\cos\theta)$ for quantum and transport relaxation rates, respectively. Using this result, Das Sarma and Stern have shown that the ratio τ_t/τ_q exceeds unity for ionized impurity scattering for both the three- and two-dimensional metallic electron gases.

Among the elastic-scattering processes, the ratio deviates strongly from unity for *Coulombic* scatterers, where the scattering potential has a long-range nature. Short-range scattering processes, such as due to alloy scattering, are isotropic, and so are inelastic-scattering processes, such as due to phonons. For such scatterers, the ratio remains close to unity. Gold[3] extended the results of Das Sarma and Stern to include interface roughness and alloy scattering in two dimensions. The two main Coulombic scattering mechanisms in semiconductors originate from randomly distributed individual charge centers (such as those from dopants, impurities, or charged vacancies) or from charged dislocations.

The problem of the ratio of transport to quantum scattering times has not yet been solved for dislocation scattering. Scattering from charged dislocations has become an increasingly important topic owing to its relevance in III-V nitride semiconductor structures. Look and Sizelove[4] recently showed the importance of charge dislocation scattering in bulk GaN. The effect of dislocation scattering on two-dimensional electron-gas conductivity was also studied.[5] Both the works calculate the transport scattering times to see its effect on electron mobilities. Many workers have reported the transport to quantum scattering time ratios for AlGaN/GaN two-dimensional electron gases (2DEG's).[6–11] These 2DEG's typically have a large number of dislocations whose effect on the quantum scattering time has not yet been studied. The recent demonstration[12] of polarization-doped degenerate three-dimensional electron gases in graded gap AlGaN/GaN structures presents another experimental system that requires a study of the ratio τ_t/τ_q for the identification of major scattering mechanisms.

In this work, we present the theory of quantum scattering times for charged dislocation scattering for both three- and two-dimensional electron gases. First, we derive a closed-form expression for the ratio τ_t/τ_q for dislocation scattering in the 3DEG. We compare the results to the case of ionized impurity scattering. We then derive the ratio for the 2DEG and compare the ratio to remote ionized impurity scattering.

We now derive an expression for the quantum scattering time of electrons for three-dimensional carriers for scattering from charged dislocations. We assume that there are N_{disl} parallel dislocations per unit area that pierce a three-dimensional electron gas of density n along the z direction. We set c to be the distance between the individual charges on the dislocation, making it a line charge of density $1/c$.

The screened Coulombic potential due to such a charged dislocation immersed in the gas of mobile carriers is given by[13]

$$V_{disl}^{scr}(r)=\frac{e}{2\pi\epsilon c}K_0\left(\frac{r}{\lambda}\right), \tag{2}$$

where K_0 is a zero-order modified Bessel function and λ is the screening length. To find the matrix element $\langle\mathbf{k}'|V_{disl}^{scr}(r)|\mathbf{k}\rangle$ for scattering, we note the fact that the scattering is two dimensional, affecting only the component of the momentum of incident electrons perpendicular to the dislocation axis, $\mathbf{k}_\perp$. Under these assumptions, the dislocation scattering matrix rate can be shown[4] to be given by

$$S_{disl}(k',k)=\frac{2\pi}{\hbar}\left(\frac{e^2}{\epsilon c}\frac{\lambda^2}{[1+(q\lambda)^2]}\right)^2\delta(E_{k_\perp}-E_{k'_\perp}), \tag{3}$$

where $q^2=|\mathbf{k}'_\perp-k_\perp|^2=2k_\perp^2(1-\cos\theta)$.

To find the quantum scattering rate, we have to sum this scattering rate for all values of $k'_\perp$ *without* the $(1-\cos\theta)$ term that is required for calculating the classical mobility.

Summing this expression over all values of $\mathbf{k}'_{\perp}$ using the prescription for two-dimensional density of states $\Sigma_{k_{\perp}}(\cdots) \rightarrow 1/(2\pi)^2 \int d^2 k_{\perp}(\cdots)$, and evaluating the integral *exactly*, we get the quantum scattering rate due to charged dislocations to be

$$\frac{1}{\tau^q_{disl}(k)} = \frac{N_{disl} e^4 m^*}{\hbar^3 \epsilon^2 c^2} \frac{\lambda^4}{(1+4k^2\lambda^2)^{3/2}} [1+2(k\lambda)^2]. \tag{4}$$

Comparing this to the transport scattering rate due to charged dislocations derived by Pödör,[14]

$$\frac{1}{\tau^t_{disl}(k)} = \frac{N_{disl} e^4 m^*}{\hbar^3 \epsilon^2 c^2} \frac{\lambda^4}{(1+4k^2\lambda^2)^{3/2}}, \tag{5}$$

we find the simple relation

$$\left.\frac{\tau_t}{\tau_q}\right|_{disl} = 1 + \frac{1}{2}\zeta^2, \tag{6}$$

where $\zeta = 2k\lambda$. For a metallic 3DEG, transport occurs between carriers at the Fermi level. Then, the scattering times can be evaluated at the Fermi energy, and $\zeta = 2k_F\lambda_{TF}$, where $k_F = (3\pi^2 n)^{1/3}$ is the Fermi wave vector and $\lambda_{TF} = q_{TF}^{-1} = \sqrt{2\epsilon\varepsilon_F/3e^2 n}$ is the Thomas-Fermi screening length, $\varepsilon_F = \hbar^2 k_F^2/2m^\star$ being the Fermi energy. Under these conditions, the lifetime ratio is dependent *only* on the carrier concentration n.

In Fig. 1, we plot the ratio of transport and quantum scattering times against the dimensionless quantity ζ. In the figure, we also plot the ratio for random impurity scattering[1] to show the relative intensity. It is seen that the ratio is more for dislocation scattering than for impurity scattering since dislocation scattering is *inherently* more anisotropic than impurity scattering. While the impurity scattering potential of point charges possesses spherical symmetry, the dislocation scattering potential of a line charge is cylindrically symmetric, thus causing an additional anisotropy in the scattering of three-dimensional carriers. The ratio approaches unity (as is also true for impurity scattering) as $\zeta \rightarrow 0$.

The transport to quantum scattering times ratio due to ionized impurities for a 2DEG has been studied in some detail in the light of experimental evidence for both Si-MOSFET metal-oxide-semiconductor field-effect transistor inversion layers and AlGaAs/GaAs modulation-doped 2DEG's. Das Sarma and Stern show in their work[1] how remote ionized impurity scattering causes the ratio to become very large as the remote donors are placed farther away from the 2DEG channel, strongly enhancing forward angle scattering. In a Si-MOSFET, the 2DEG is formed by inversion induced by a gate voltage. In a AlGaAs/GaAs heterojunction, the 2DEG is formed by intentional modulation doping from remote donors.

An AlGaN/GaN 2DEG is distinct from these cases, where the 2DEG forms due to the strong internal polarization fields[15] that extract carriers from remote surface states.[16] There is no intentional doping for these structures, and scattering originates from the donor-like surface states that supply the 2DEG electrons. Thus, the distance of the remote donors from the 2DEG is fixed by the AlGaN layer thickness. We calculate the relaxation rate ratio for remote ionized impurity scattering for such a structure with a changing AlGaN layer thickness; the results are shown in Fig. 2. As is easily seen, the ratio becomes much larger than unity as the AlGaN layer thickness increases. We will briefly compare this result with the case of charged dislocation scattering.

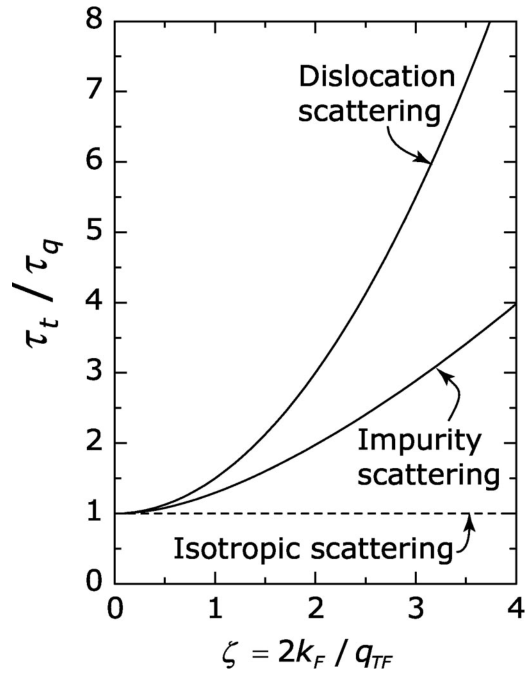

FIG. 1. Plot showing the lifetime ratio for scattering from charged dislocations and ionized impurities for a degenerate electron gas as a function of the carrier density. The ratio deviates significantly for the two Coulombic scattering processes from the normal value of unity for all other non-Coulombic isotropic scattering processes. The plot is generated from the *exact* relations for the lifetime ratio for the two scattering mechanisms derived in this work.

The transport scattering rate due to charged dislocation scattering for 2DEG carriers was derived recently.[5] The screened matrix element for charged dislocation scattering was derived to be

$$\langle k' | V(r) | k \rangle = \frac{e}{\epsilon c} \frac{1}{q(q+q_{TF})}, \tag{7}$$

where q_{TF} is the two-dimensional Thomas-Fermi screening wavevector and $q = |\mathbf{k}' - \mathbf{k}| = 2k_F \sin(\theta/2)$ is the change in the 2D wavevector due to scattering. Using this result, we derive the quantum scattering rate to be

$$\frac{1}{\tau_q} = \frac{N_{dis} m^* e^2}{\hbar^3 \epsilon^2 c^2} \frac{I_q}{4\pi k_F^4}, \tag{8}$$

where I_q, an integral dependent on the dimensionless parameters ζ and $u = q/2k_F = \sin(\theta/2)$ (θ is the angle of scattering), is given by

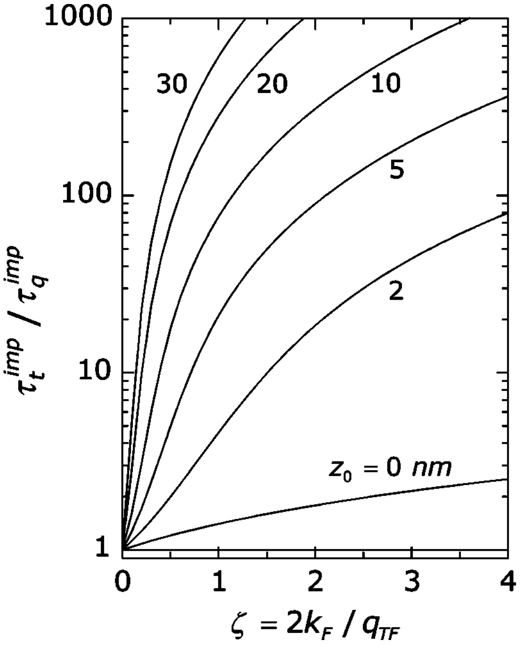

FIG. 2. Plot showing τ_t / τ_q for scattering from remote impurities for an AlGaN/GaN two-dimensional electron gas. The different curves are for changing thickness of the AlGaN barrier. The ratio increases very fast with the barrier thickness, since remote impurity scattering strongly enhances small-angle scattering, increasing the transport scattering time.

$$I_q = \frac{1}{2}\zeta^2 \int_0^1 du \frac{1}{u^2(1+\zeta^2 u^2)\sqrt{1-u^2}}. \tag{9}$$

The transport scattering rate is given by

$$\frac{1}{\tau_t} = \frac{N_{dis} m^* e^2}{\hbar^3 \epsilon^2 c^2} \frac{I_t}{4\pi k_F^4}, \tag{10}$$

where I_t is given by

$$I_t = \zeta^2 \int_0^1 du \frac{1}{(1+\zeta^2 u^2)\sqrt{1-u^2}}. \tag{11}$$

Whilst I_t can be evaluated exactly, it can be easily seen that I_q *diverges* as $u = \sin(\theta/2) \to 0$, or, in other words, when $\theta \to 0$. This is the case of scattering that is strongly peaked in the forward direction. The ratio of the quantum and transport scattering times, given by the ratio τ_t / τ_q, thus acquires a singularity at small scattering angles. We define a scattering angle cutoff θ_c and evaluate the ratio τ_t / τ_q by including dislocation scattering restricted to $\theta \geqslant \theta_c$ only. We evaluate the ratio for the cutoffs $\theta_c = \pi/10, \pi/100, \pi/1000, \pi/10\,000$. The results are shown in Fig. 3.

As more small-angle scattering contribution is included, the ratio becomes much larger than unity. On the other hand, as the scattering is restricted to be more large angle, the ratio approaches unity since it mimics isotropic scattering. Two points can be made about the results. First, that the dependence of the ratio on the 2DEG density is much weaker than for impurity scattering (Fig. 2). Second, that the ratio is much larger than that for impurity scattering as $\theta_c \to 0$.

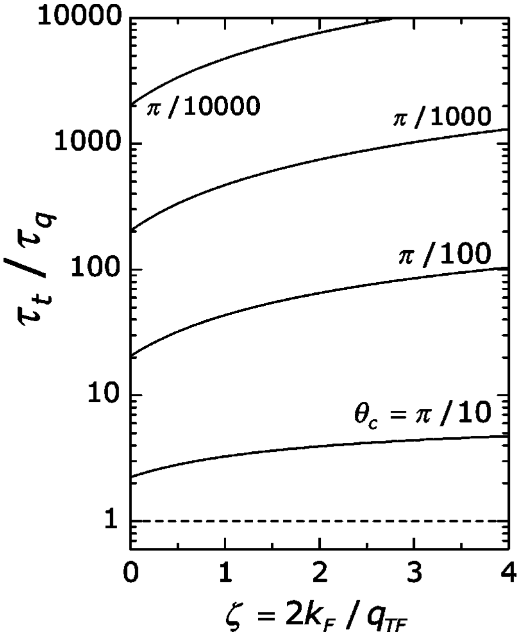

FIG. 3. Plot showing τ_t / τ_q for scattering from charged dislocations for a 2DEG. The different curves are for different small-angle cutoffs θ_c for scattering as treated in the paper. As more small-angle scattering is included, the ratio becomes very large and eventually diverges as $\theta_c \to 0$. The dependence of τ_t / τ_q is much weaker for dislocation scattering than impurity scattering for 2DEG's.

One can argue that as opposed to the case of impurity scattering for 2DEG's, where the modulation dopants can be placed at any distance from the 2DEG, a charged dislocation line *always* has a strong *remote impurity* nature due to the geometry. This causes a strong preference for small-angle scattering, causing the ratio $\tau_t / \tau_q \to \infty$ as $\theta_c \to 0$. Our model of dislocation scattering implies that quantum scattering from dislocations should have a *minimal effect* on the broadening of Landau levels, which in all likelihood will be determined by other scattering events. We point out here that such a divergence of the quantum scattering time for a 2DEG was also observed by Gold[3] for the case of residual impurity scattering. In his work, by considering the multiple-scattering events contribution to the self-energy in the Green's function, he was able to arrive at a renormalized quantum scattering time, which removed the singularity. This kind of a treatment for dislocation scattering in 2DEG's might be an interesting application of many-body theoretical techniques, which we do not attempt here.

Finally, we mention that the scattering time ratio is independent of the density of scatters. However, if one measures τ_t from the mobility and τ_q from the amplitudes of Shubnikov–de-Haas oscillations, one measures the scattering time determined by the dominant scattering mechanism. That of course depends on the density of the scatterers. Hsu and Walukiewicz have recently shown that the ratio τ_t / τ_q for AlGaN/GaN 2DEG's is the largest when *both* long- and short-range scattering mechanisms contribute to the total scattering. The analysis of experimentally determined τ_t / τ_q

ratios in AlGaN/GaN 2DEG's needs to include the effect of a *large* increase in the ratio due to the effects of dislocation scattering. The recently demonstrated polarization-doped three-dimensional electron gases[12] provide an ideal testing ground for applying our results for the 3DEG case. By exploiting the internal polarization fields, wide degenerate electron slabs of high mobility were demonstrated in the graded AlGaN material system. The 3DEG densities in such electron slabs are in principle, tunable over a wide range 10^{16}–10^{18} cm^{-3}. Besides, the carriers do not freeze out at low temperatures and have been shown to exhibit Shubnikov–de Haas oscillations.[17] Such degenerate 3DEG's typically have a high density of dislocations ($N_{disl} \approx 10^9$ cm^{-2}) and should be an ideal testing ground for our theoretical predictions.

In summary, we derived the transport to quantum scattering times for dislocation scattering for the three- and two-dimensional electron gases. We compared the results to impurity scattering and found the effect to be stronger for dislocation scattering for both cases. We attribute this to the inherent anisotropy in scattering events due to the geometry of dislocations. We point out experimental systems where our results will prove helpful.

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