

Investigation of the Dyakonov-Shur instability for THz wave generation based on the Boltzmann Transport Equation

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Abstract. We compute the growth rate of the Dyakonov-Shur plasma instability of a quasi 2D electron gas by numerical simulations based on the Boltzmann transport equation. We present a method to solve the characteristic equation by a Newton approach to find the two Vlasov modes. A deterministic solver using Fourier harmonics in the 2D $\mathbf{k}$ -space is applied to carrier transport in the framework of the Dyakonov-Shur model. We investigate the suppression of the plasma growth rate due to the Pauli principle and temperature.

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1. Introduction

The part of the electromagnetic spectrum which lies between microwaves and infrared light is sometimes referred to as the THz gap due to the lack of high power sources and sensitive devices to emit and detect THz waves [1]. A promising approach to generate THz radiation is based on plasma waves in semiconductor devices [2–5]. One of the possible mechanisms was suggested by Dyakonov and Shur, who noticed that a steady current in a submicron gate-length Field Effect Transistor (FET) with asymmetric boundary conditions can become unstable and generate plasma waves [6, 7]. Plasma waves propagate at a speed which is much higher than the electron drift velocity, and devices utilizing plasma waves can operate at higher frequencies than conventional transit time limited devices [8]. The frequency can reach the THz range by choosing sufficiently short gate lengths and high electron concentrations [9].

The theoretical modeling of plasma waves in FETs developed by Dyakonov-Shur was based on the first two moments of the Boltzmann Transport Equation (BTE), which are the continuity and Euler equations [7, 10]. To avoid strong damping, the mean free path of the electrons should be larger than the channel length of the FET resulting in quasi ballistic transport; making modeling with two moments difficult. Due to the high sheet density the Fermi energy lies above the lowest subband and the Pauli principle can no longer be neglected. Therefore, the accuracy of a moment-based approach which does not contain the Pauli principle is questionable. In Ref. [11] it is shown that the simple transport model of Ref. [6] fails to capture important aspects of transport not only in the case of strong non-equilibrium but also in the linear response regime at equilibrium for high frequencies and large wave numbers. Therefore, solving the BTE is always more accurate than moments-based approaches [12, 13]. Since the transport in a real semiconductor device is damped and the Pauli principle is important, the BTE with particle scattering (e.g. electron phonon scattering) has to be solved rather than the collision less one [14].

The calculation of plasma waves based on the Euler equation gives a plasma dispersion relation with two branches. They propagate upstream and downstream w.r.t. the electron current and are usually called Vlasov modes. The BTE yields in addition a continuum of modes [15]. In the case of a numerical solution of the BTE for each variable of the corresponding discrete system a plasma mode is obtained [16]. At small electric fields and low frequencies the two modes with the least damping are well separated from the others w.r.t. damping and can consequently propagate further than the other modes. It is easy to identify these two modes as the Vlasov modes. On the other hand, in the case of strong non-equilibrium and high frequencies identification of the two Vlasov modes by simple means is no longer possible [16]. In this case the assumption of only two plasma modes fails and the transport model has to be solved numerically in the real space, which is not done in this work. Instead, in this work the Dyakonov-Shur approach based on two plasma modes is extended to the case of the full Boltzmann equation. In the next section we show how to do this. In the results section we demonstrate the impact of the Pauli principle and temperature.

2. Modeling

In order to follow the Dyakonov-Shur approach [6], we consider a double gate structure with a homogeneous quasi-2D electron gas located in the plane at $z = 0$. The channel is sandwiched between two oxide regions with dielectric constant ϵ_{ox} and thickness d_{ox} . Moreover, the quasi-2D electron gas is assumed to be thin compared to the oxide thickness. The highly conducting gate contacts with zero thickness are placed at $z = \pm d_{\text{ox}}$ on the surface of the oxide regions (Fig.1). The gate voltage controls the electron density within the quantum well and the electron velocity is regulated by applying a homogeneous stationary electric field along the channel. To study plasma wave propagation, Dyakonov and Shur assumed that there is a stationary state in which

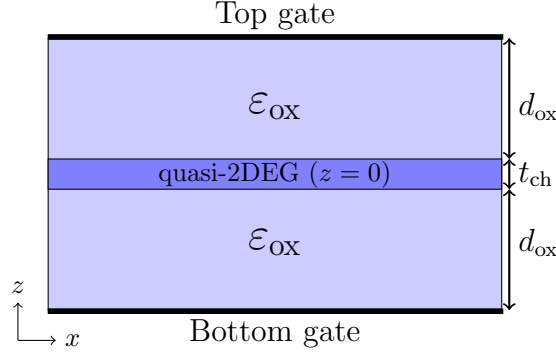


Figure 1. A symmetric double gate structure with a quasi-2D electron gas at $z = 0$, which is assumed to be very thin and sandwiched between two thick oxide layers with metal gates.

the plasma parameters are uniform and constant in time [6, 8]. Then the time and position dependencies of the parameters are investigated at a small deviation from this stationary state. It is thus supposed that the linear response of the transport model is sufficient and all variables are expanded up to the first order in a harmonic function in both time and space around the stationary state $\tilde{A}$ [11, 16]

$$A(x, t) = \tilde{A} + \Re\{\underline{A} \exp(-j\underline{q}x + j\underline{\omega}t)\} \quad (1)$$

where $\underline{A}$ is the phasor of the small-signal quantity for the complex angular frequency $\underline{\omega}$ and wave number $\underline{q}$, and $\tilde{A}$ its stationary value.

Our approach to get the steady state solution involves solving the Poisson equation (PE) for the electrostatic potential in the 2D real space and the Schrödinger equation in confinement direction self-consistently to get the desired DC electron density by adjusting the gate voltage. Then the BTE is solved deterministically using the Fourier harmonics expansion in transport direction [17]. Numerical experiments show that a Fourier harmonics expansion of the third order is sufficient for this case and will be used in all simulations.

In accordance with the Dyakonov-Shur model the PE is solved for plasma waves in x direction assuming a homogeneous system in that direction. The analytical solution of the linearized PE with a Dirichlet boundary condition at the top and bottom gates is given by

$$\underline{\varphi}(z) = \frac{e\underline{n}}{2\varepsilon_{\text{ox}}\underline{q}} \left(\sinh(\underline{q}|z|) - \tanh(\underline{q}d_{\text{ox}}) \cosh(\underline{q}|z|) \right), \quad (2)$$

where e is the positive elementary charge and $\underline{n}$ the small-signal electron sheet density of the quasi-2D electron gas assuming that the spread of the electron density in z direction is negligible. We use $\tanh(\underline{q}d_{\text{ox}}) \approx \underline{q}d_{\text{ox}}$ under the assumption that $\underline{q}d_{\text{ox}} \ll 1$ [6]. With these assumptions, only the small-signal electric field $\underline{E}$ in x direction at $z = 0$ is required

$$\underline{E}_x = j\underline{q} \underline{\varphi}(z = 0) = -j\underline{q} \frac{e\underline{n}d_{\text{ox}}}{2\varepsilon_{\text{ox}}}. \quad (3)$$

The electron sheet current density is given with the conductivity by

$$\underline{J}_x = \underline{\sigma} \underline{E}_x, \quad (4)$$

where the small-signal conductivity includes the drift and diffusion terms and depends on $\underline{\omega}$ as well as $\underline{q}$ and can be evaluated by the BTE. With this the continuity equation

$$-e\underline{j}\omega \underline{n} - \underline{j}q \underline{J}_x = 0, \quad (5)$$

yields the characteristic equation for plasma waves, of which the plasma dispersion $q(\underline{\omega})$ is the solution [16]:

$$1 + \underline{q}^2 \frac{d_{\text{ox}}}{2\underline{j}\omega \varepsilon_{\text{ox}}} \underline{\sigma}(\underline{\omega}, \underline{q}) = 0. \quad (6)$$

The small signal BTE is linearized, discretized and solved based on the methods which are described in detail in Refs. [16,17]. The dependency of the small-signal conductivity (4) on the complex angular frequency and wave number is directly calculated by the solution of the discrete small-signal BTE:

$$\underline{\sigma} = \frac{\underline{J}_x}{\underline{E}_x} = \frac{\vec{c}_J^T \vec{f}}{\underline{E}_x}, \quad (7)$$

where $\vec{c}_J$ projects the vector of the small-signal distribution function $\vec{f}$ onto the current density and does not depend on $\underline{q}$ or $\underline{\omega}$.

In order to solve the characteristic equation (6) by a Newton approach, the derivative of the small-signal conductivity w.r.t. $\underline{q}$ and $\underline{\omega}$ has to be calculated:

$$\frac{\partial \underline{\sigma}}{\partial \underline{\omega}} = \vec{c}_J^T \frac{\partial}{\partial \underline{\omega}} \frac{\vec{f}}{\underline{E}_x}, \quad \frac{\partial \underline{\sigma}}{\partial \underline{q}} = \vec{c}_J^T \frac{\partial}{\partial \underline{q}} \frac{\vec{f}}{\underline{E}_x}. \quad (8)$$

This can be done in a straightforward manner, because the small-signal BTE leads to a linear system of equations which can be written in the form [16]:

$$\left[\underline{j}\omega \hat{D} - \underline{j}q \hat{B} + \hat{C} \right] \frac{\vec{f}}{\underline{E}_x} = \vec{b}, \quad (9)$$

where $\hat{D}$, $\hat{B}$ and $\hat{C}$ are real valued matrices which do not depend on $\underline{\omega}$ and $\underline{q}$. The vector $\vec{b}$ is related to the stationary distribution function. The corresponding derivatives of the small-signal distribution can then be found by solving the linear equation systems of:

$$\begin{aligned} \left[\underline{j}\omega \hat{D} - \underline{j}q \hat{B} + \hat{C} \right] \frac{\partial}{\partial \underline{\omega}} \frac{\vec{f}}{\underline{E}_x} &= -\underline{j}\hat{D} \frac{\vec{f}}{\underline{E}_x} \\ \left[\underline{j}\omega \hat{D} - \underline{j}q \hat{B} + \hat{C} \right] \frac{\partial}{\partial \underline{q}} \frac{\vec{f}}{\underline{E}_x} &= \underline{j}\hat{B} \frac{\vec{f}}{\underline{E}_x}. \end{aligned} \quad (10)$$

With these derivatives the characteristic equation (6) is solved by the Newton method for the dispersion relations of the upstream and downstream modes. The calculation starts with zero stationary electric field in the channel, for which the two Vlasov modes can be easily identified. Then the electric field is increased by sufficiently small amounts such that in the Newton iteration jumping to different modes can be avoided. By this

approach it is possible to follow both branches of the dispersion relation up to high stationary electric fields.

Self-excitation of plasma oscillations in the channel of the FET can lead to the emission of THz radiation. The proposed mechanism by Dyakonov-Shur for the plasma instability is based on the reflection of plasma waves by the transistor boundaries with enhanced amplitudes [6]. This condition requires asymmetric boundary conditions at the source and drain side of the channel. The choice made by Dyakonov and Shur was a grounded source contact (zero small-signal electron density at $x = 0$) and open drain contact (zero small-signal current density at $x = L$). Superposition of two waves (one upstream $\underline{q}^+(\underline{\omega})$ with $\Re\{\underline{q}^+\} > 0$ and one downstream $\underline{q}^-(\underline{\omega})$ with $\Re\{\underline{q}^-\} < 0$) results for the small-signal electron density in

$$\underline{n}(x) = \underline{n}^+ \exp(j\underline{q}^+(\underline{\omega})x) + \underline{n}^- \exp(j\underline{q}^-(\underline{\omega})x) , \quad (11)$$

where $\underline{q}^+$ and $\underline{q}^-$ are the wave numbers of the two Vlasov modes in a homogeneous channel of length L for the complex angular frequency $\underline{\omega}$, which are solutions of the characteristic equation. Applying the source boundary condition $\underline{n}(0) = 0$ to the linear combination yields $\underline{n}^- = -\underline{n}^+$. The drain boundary condition for the current density $\underline{J}_x(L) = 0$ results in [18]:

$$\underline{q}^+(\underline{\omega}) \exp(j\underline{q}^+(\underline{\omega})L) - \underline{q}^-(\underline{\omega}) \exp(j\underline{q}^-(\underline{\omega})L) = 0 . \quad (12)$$

This equation is again solved by the Newton method, which yields the corresponding $\underline{\omega}$ for a given stationary electric field. The calculation starts at zero stationary electric field, for which the wave numbers are given by $\underline{q}^+ = -\underline{q}^- = \pi/2L$. In this case the characteristic equation is solved for $\underline{\omega}$ and these values are used to start the calculation for nonzero electric fields. Again, sufficiently small increases of the electric field are used to avoid changes in the plasma wave modes.

3. Results

Results are presented for the device depicted in Fig.1 with a $t_{\text{ch}} = 5\text{nm}$ thick lowly doped channel and oxide thickness of $d_{\text{ox}} = 20\text{nm}$. The oxide permittivity is set to be the same as the GaAs permittivity $\epsilon_{\text{ox}} = \epsilon_{\text{sc}} = 12.9\epsilon_0$. The quasi-2D electron gas has a density of $2 \times 10^{12}\text{cm}^{-2}$ which leads to a degenerate electron gas. A grid spacing of 0.25nm is used in the confinement direction for the self-consistent solution of the PE and Schrödinger equation under stationary conditions. An equi-distant grid spacing of 3meV is used in energy space. In transport direction is assumed the device is homogeneous with a channel length of $L = 60\text{nm}$. The subbands included in the BTE are limited to the 8 lowest ones. A non-parabolic conduction band structure is considered for GaAs which comprises the Γ -valley, four equivalent L-valleys and three equivalent X-valleys. Intra-valley elastic acoustic phonon, inter-valley phonon scattering and intra-valley polar optical phonon scattering are included in the scattering term [19,20]. We use the material parameters reported in [21] for GaAs. The interface between GaAs and the oxide is assumed to be smooth.

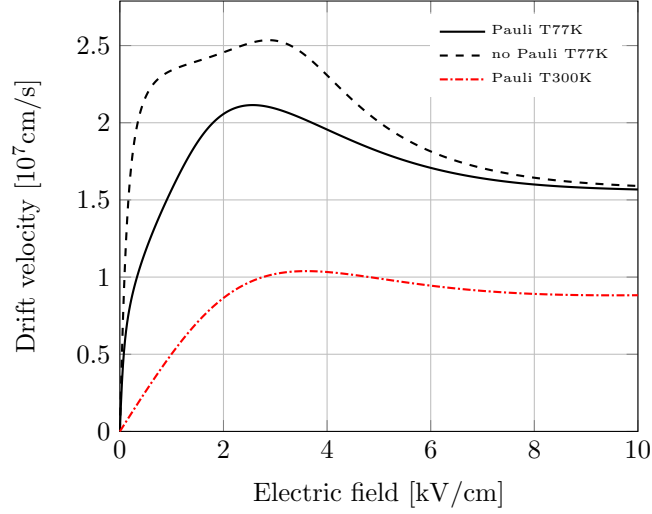


Figure 2. Electron drift velocity as a function of the stationary electric field for the GaAs FET including (solid line) and excluding the Pauli principle (dashed line) at 77K and 300K (red line).

Pauli	T(K)	μ_0 (cm ² /Vs)
With Pauli	300	5.27×10^3
With Pauli	77	9.02×10^4
Without Pauli	77	1.29×10^5

Table 1. Low-field mobility μ_0 for GaAs

For the Dyakonov-Shur instability it is essential that the plasma velocity is larger than the electron drift velocity. On the other hand, another major requirement to obtain plasma emissions in the THz regime is that the electron drift velocity should not be much smaller than the plasma wave velocity [6]. The relation between the velocity and electric field for high mobility materials such as GaAs shows a velocity overshoot. Thus, electrons can reach rather high velocities.

Fig. 2 shows the velocity-field characteristics of a FET with a GaAs quantum well. At low electric fields, most of the electrons are in the Γ -valley and the drift velocity increases with higher fields. A further increase of the electric field leads to a negative differential mobility because electrons begin to occupy the higher valleys. Since the L- and X-valleys have much higher effective masses and their scattering rate for intervalley scattering is larger than in the Γ -valley, the drift velocity is reduced [22].

By reducing the temperature the phonon occupation number following Bose-Einstein statistic is lowered. Thus the scattering rate decreases and consequently the low field mobility, the saturation velocity and the velocity overshoot increase. Table 1 shows the low field mobility for the different cases of Fig. 2.

GaAs has a low density-of-states mass because of the small effective mass of the lowest valley (Γ -valley). Thus, for such a high electron sheet density, the Fermi energy

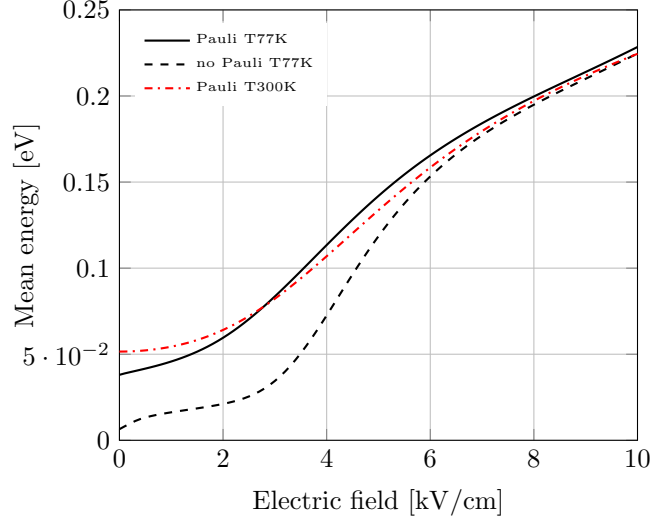


Figure 3. Electron mean energy as a function of the stationary electric field for the GaAs FET at 77K including (solid line), and excluding the Pauli (dashed line) line, and 300K(red line)

($E_f = -0.158\text{eV}$) lies above the minimum of the lowest subband($E_s = -0.231\text{eV}$) and the Pauli principle cannot be neglected. The Pauli principle limits the occupancy of the states to a single electron per spin direction thus electrons are pushed to higher energies at lower electric fields, where scattering is stronger (Fig. 3).

The complex angular frequency is defined as $\underline{\omega} = \omega' - j\omega''$, where the real part ω' is the oscillation frequency and the imaginary part ω'' is the growth rate of the plasma wave. To find $\underline{\omega}$ for a real-valued q , the characteristic equation is solved resulting in multiple solutions where the number of solutions matches the number of variables in the discrete BTE. Fig. 4 shows some of the modes close to the origin at zero stationary electric field. In this case the wave number of the Dyakonov-Shur instability is $\underline{q}^+ = -\underline{q}^- = q = \pi/2L$ corresponding to a quarter wavelength of a standing wave in the channel. Due to the equilibrium condition, the distribution of the modes is symmetric and two modes with the smallest $|\omega''|$ and $|\omega'| > 0$ are clearly separated from the others. The one with positive ω' together with $\underline{q}^+ = -\underline{q}^- = \pi/2L$ is selected as the starting point for the calculation of the Dyakonov-Shur instability as a function of the stationary electric field.

The growth rate of the plasma oscillation is characterized by ω'' ; for $\omega'' > 0$ the device becomes active. In Fig. 5 the real and imaginary part of the complex angular frequency are plotted as a function of the drift velocity, which in turn is a function of the stationary electric field. As we can see at low drift velocities, the growth rate ω'' depends linearly on the drift velocity. With increasing drift velocity it grows monotonically up to a maximum value, after which it quickly falls off. As a result of this, in the case of $T=77\text{K}$, ω'' is only positive in a finite range of drift velocities. If the Pauli principle is excluded, the mobility is overestimated which in turn leads to a significant overestimation of the growth rate. At 300K the plasma oscillation can not become

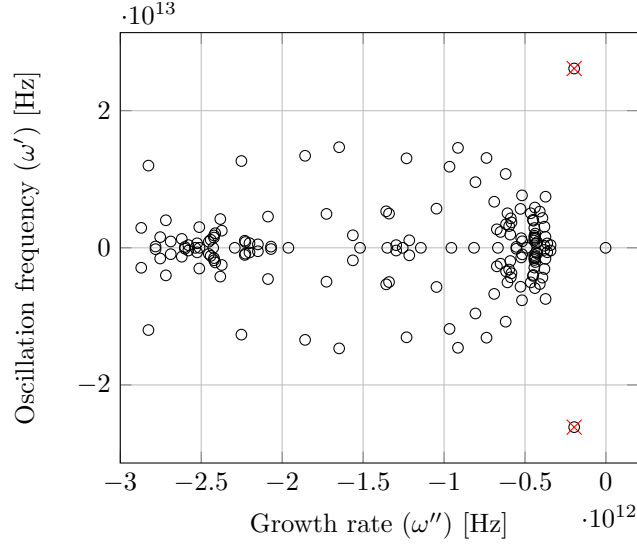


Figure 4. Complex angular frequency ($\underline{\omega}$) of plasma modes close to the origin for $q = \frac{\pi}{2L}$ at zero electric field and 77K including the Pauli principle. The two red symbols $\times$ point to the modes with the smallest $|\omega''|$ and nonzero oscillation frequency.

active, because of the low electron mobility, which is due to the stronger electron-phonon scattering. The ensuing strong dissipation leads to damping of the plasma waves resulting in a reduction of the growth rate.

As opposed to the growth rate, the oscillation frequency ω' shows only a minor dependency on the drift velocity, where with increasing drift velocity, ω' slightly falls.

In Fig. 6, the real and imaginary part of the wave number are plotted versus the drift velocity for the corresponding complex angular frequencies from Fig. 5 including the Pauli principle at 77K. As previously mentioned, the upstream and downstream wave numbers for each drift velocity are chosen among a multitude of modes using the Newton method. Up to a critical drift velocity, the two modes with the lowest absolute value of the imaginary part of q can clearly be separated from the others. Since these modes have the least amount of damping, they can propagate further than the other modes [16]. In Fig. 7 the wave numbers of the modes close to the origin are plotted for a drift velocity of $v_D = 1.7 \times 10^7 \text{ cm/s}$ for which the maximum growth rate is achieved. For this drift velocity the two Vlasov modes are still distinguishable from the rest of the modes. The complex angular frequency is calculated up to the overshoot velocity since finding the correct q among multitude modes for $\underline{\omega}$ becomes difficult beyond this velocity.

4. Conclusion

We simulated the Dyakonov-Shur plasma instability by a deterministic solver for the BTE which includes electron-phonon scattering and the Pauli principle. The resultant numerical solution of the BTE contains a multitude of modes, of which the two modes

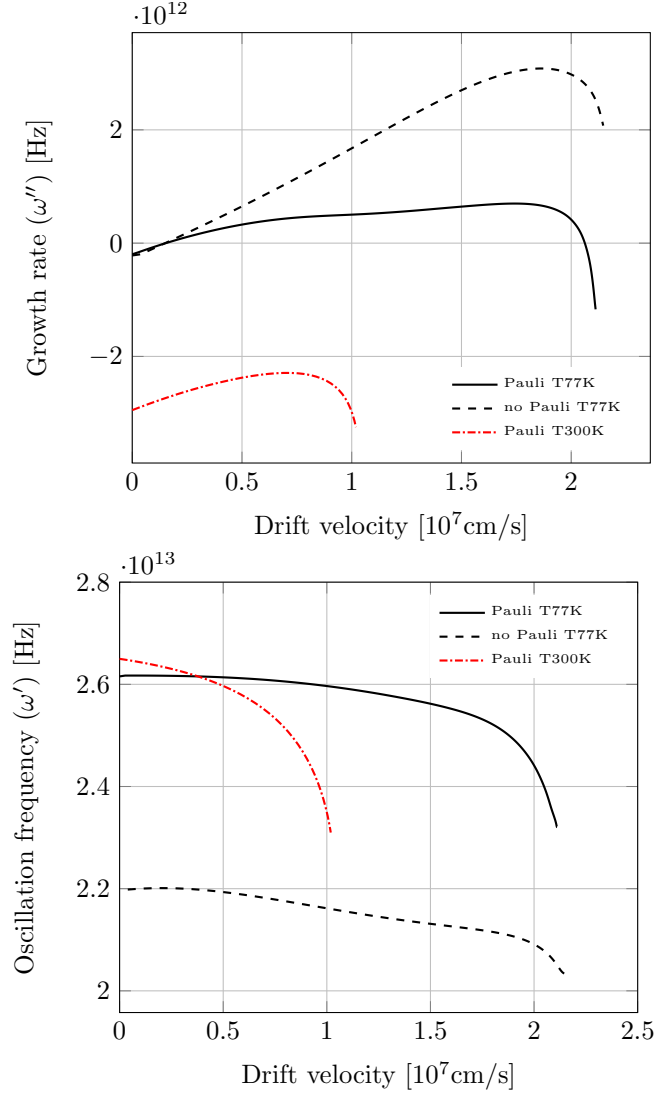


Figure 5. The imaginary (growth rate) and real (oscillation frequency) part of the complex angular frequency versus drift velocity.

with the least damping can be identified as the Vlasov modes up to a critical electric field by a Newton method.

We were able to investigate the impact of the Pauli principle on plasma waves, which is not possible by the typical moments-based methods which do not contain it. At high electron densities, where the Pauli principle has a strong effect on the electron distribution function, the growth rate of the Dyakonov-Shur instability is strongly reduced compared to the calculation without the Pauli principle.

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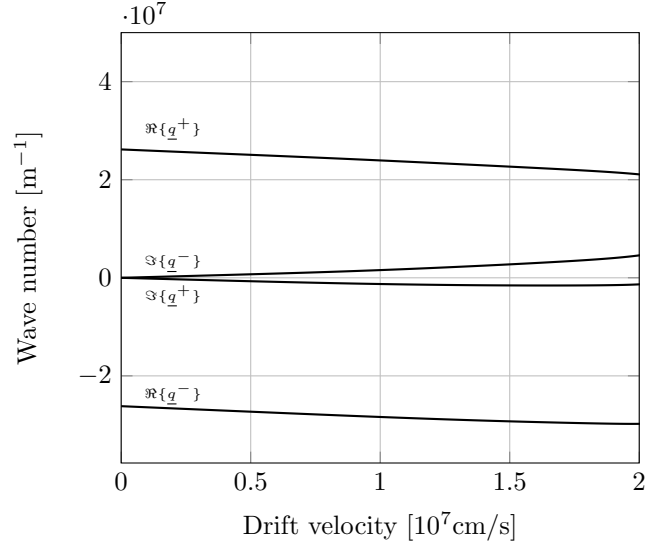


Figure 6. The upstream and downstream wave numbers corresponding to the complex angular frequencies shown in Fig. 5 versus the drift velocity including the Pauli principle at 77K.

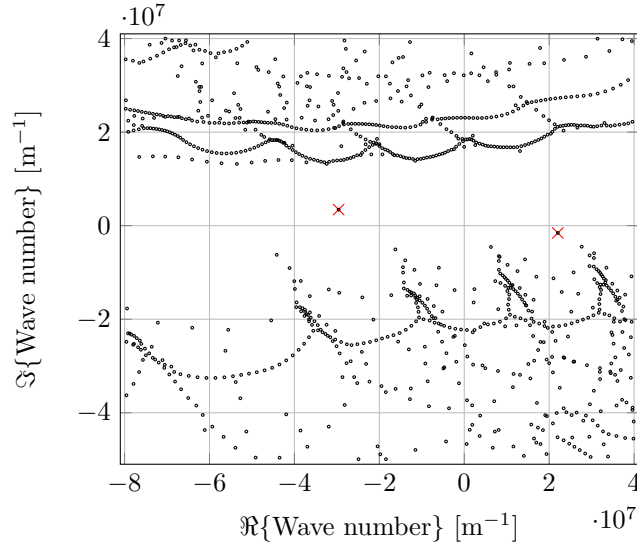


Figure 7. Modes close to the origin including the Pauli principle at 77K for a drift velocity of $v_D = 1.7 \times 10^7 \text{ cm/s}$ which leads to the maximum growth rate (ω'') shown in Fig.5. The two modes which are highlighted by $\times$ are the two Vlasov modes which were found using the Newton method.

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