Microwave Noise in Semiconductor Devices

Module 7

Austin J. Minnich, California Institute of Technology

Spring Term 2020

1 Microscopic description of electron transport and fluctuations

We have obtained a high-level understanding of the phenomenology of hot electron noise from the previous macroscopic treatment. Now, we'd like to develop a microscopic treatment of electronic transport and fluctuations at the level of electronic states and transition rates due to scattering. For that, we need to dive further into the equations governing the evolution of the occupation of electronic states, the Boltzmann equation.

2 Boltzmann equation (BE)

The Boltzmann equation is a partial differential equation for the single-particle occupancy function in momentum space ( ) and real space ( ) at different instants in time ( ) while the system is subject to real space gradients, external fields, and scattering. It mathematically expresses the intuitive concept that the volume of phase space is preserved under the above perturbations. It reads:

There are several ways to derive the BE that I won't go through in the full detail.

2.1 Classical derivation highlights

From only the concept that a phase space for an N-particle system exists, the Liouville theorem can be derived. It says that the volume of phase space of the N-particle system is preserved in the absence of dissipation. The corresponding N-particle distribution function

obeys a continuity equation like that for mass conservation of fluid flows, for example. There is no scattering term in this equation since it is for the full N particle system!

From this, we can compute the one-particle distribution function by integrating out the other N-1 degrees of freedom. The equation for will depend on the two-particle distribution function . From here, we can make the "molecular chaos" assumption (Stosszahlansatz) that . This assumption yields the BE which in this form is a partial differential equation with a nonlinear collision integral.

2.2 Quantum derivation highlights

Nedjalkov, Querlioz, Dollfus, Kosina Chap 5

Start with the von Neumann equation for the density matrix of a pure state. Change variables to a center of mass frame, .

Obtain an equation for the Wigner function by Fourier transforming this equation with respect to . We now have an equation on a phase space in variables .

This is not quite the BE because the Wigner function can be negative. Assume the potential is at most quadratic in spatial coordinate. Then the dynamics of the Wigner function are identical to those of classical dynamics. If the distribution starts all positive it will remain so as under classical evolution.

Include an electron-phonon interaction term in the Hamiltonian to get a collision integral (otherwise we get a collision-less BE). Assume weak coupling and trace out the phonon system. Assume time scales are long compared to collision time to get a bunch of delta functions that allow the interaction term to reduce to Fermi's golden rule.

Now consider that the collision integral has been linearized so that it is given as a matrix. The desired solution is a vector of unknown occupancies of the electronic states. Then the BE is nothing more than a set of partial differential equations governing the occupancy of the single-particle states.

The collision integral will look something like this:

The diagonal terms represent the net rate of population loss out of that state. The off-diagonal terms describe in-scattering from the column state to the row state.

A well-behaved collision integral must have the columns summing to zero since scattering probabilities must conserve particles.

2.3 Validity of BE

The validity of the BE to describe transport in space and time is subject to quasi-classical restrictions. Specifically the change of on the scale of the de Broglie wavelength must be sufficiently small. In math, where is the characteristic length of the variation in .

Also, if is the characteristic energy variation in , we need the frequencies of interest .

Another fundamental assumption is that the time between successive scatterings, , is much bigger than the duration of individual scattering times, .

More precisely: the time in which two particles are within an interaction distance of radius is , where is the particle's velocity, is the interaction distance so that is the collision cross-section. From gas kinetics, we know , where is the number density of particles, .

The ratio is the gas parameter: . So we need mean distance between particles much bigger than their characteristic dimension → low density gas.

These requirements are all usually met for free electrons in a doped semiconductor.

2.4 Observables

If the distribution function is known, all other observable quantities can be obtained. For instance, the particle density at a give location at time is:

The particle flux is

Example: We can show that the BE conserves particles. Let's sum the BE over momentum (summing the columns of the matrix equation) to get an equation for the particle density . We get

This can be rewritten as

which we see is the standard conservation equation, in this case for the particle number density.

Now let's get some intuition for the Boltzmann equation.

2.5 Warmup #1: relaxation time approximation

Consider a homogeneous electron gas subject to an external electric field. We want to solve for the steady-distribution that arises due to the field. Let's make the relaxation time

approximation (RTA) that the collision integral is written as:

In the RTA form, we can more clearly see the meaning of the diagonal elements of the collision matrix - they represent a characteristic time for a state to lose population to other states and thereby return to the equilibrium distribution.
Explicitly, say the population for some state starts at some non-equilibrium value. The differential equation governing the time evolution of the state is (neglecting any fields)

The solution is just

So we see that the distribution relaxes to the value over characteristic time .
Now consider the BE for the steady distribution with a field, under the RTA.

We can write the solution simply as

Now let's compute the electric current density:

Using Ohm's law, , we see that we have derived an expression for the electrical conductivity in terms of microscopic parameters of the electronic states.

2.6 Warmup #2: Davydov distribution (Kogan)

Now let's consider the case when electrons can get far away from equilibrium. This problem was originally considered by Russian physicist Davydov in 1935.

The problem is to obtain the steady distribution of electrons subject to a field and scattered in a quasi-elastic manner such that the momentum distribution of the electrons is isotropic in momentum space.

Let's write the Boltzmann equation for this case:

For a uniform, isotropic conductor with a field applied along some direction, depends only on two variables, , where is the effective mass; and where is the angle between and applied field .

Generally, we can expand a function in 3D (momentum space) in Legendre polynomials:

The expansion coefficients are , depending on energy. If no current exists, all except .

The current can be expressed just using . The reason that we only need that term is that current along the field axis has a factor , which equals . Since Legendre polynomials are orthogonal, integrating out the angle variable to compute the current kills off all other terms except that proportional to .

Also, since , we know is the electron distribution in energy as it lacks any angular dependence in momentum space. If no current flows, then

Here is the chemical potential, is the lattice (phonon) temperature.

Following our earlier discussion on quasi-elastic scattering, we are making the assumption that the momentum space distribution is nearly isotropic. That means the only anisotropy is arising from the field and that we therefore only need to keep . [Original approx due to Pidduck (1916) and Davydov (1935,36,37)] We can solve the BE by expanding the equation in spherical harmonics and solving at each order. The collision integral is given simply as a sum of , independent of , and where is the momentum relaxation time.

Let's get the equation for first. Consider the rate of change of the number of electrons in a thin spherical shell in momentum space from . It equals

where is the density of states.

This rate must be equal to the flux of electrons (in momentum space) at energy . We therefore see that

We know the expression for electron flux:

The probabilities of emission and absorption of a phonon per time are . They have the ratio

Since we know the scattering is quasi-elastic, we use

Then we get

with the inverse energy relaxation time:

$$\frac{1}{\tau_0(E)} = \frac{1}{E}\int_0^E dE \sum_{k'} \Theta(E(k') - E) W_{abs}(kk')\hbar\omega(k' - k)/k_B T_0 \quad (1)$$

Multiply by and integrate to get two equations:

A 'temperature' of electrons is introduced:

Integrating the second equation gives the Davydov equation in energy:

In the homework, you will compute this distribution and see how it looks.

3 Fluctuations from a non-equilibrium steady state

Now to the hard part. How can we describe current fluctuations in an electron gas acted on by an electric field - in other words, fluctuations from a non-equilibrium steady state? This problem has been considered over many years as described in the previous module.

I want to first describe why fluctuations in population and hence current occur in the first

place. The BE describes the mean occupancy of a given state. The collision matrix describes the mean rate of transfer of population from one state to another.

However, the scattering process is a shot-type process - in any given time instant, there is a probability for the scattering event to occur. The probability is independent of whether other scattering events did in fact occur. This situation is exactly analogous to the shot noise process we considered at the beginning of class. The rate of population transfer therefore has a variance, about the mean, that is proportional to the mean transfer rate! At any given time instant, these population transfers might not be precisely balanced (although on average, they are). That implies that a source of fluctuations exists, regardless of value of the distribution function at any time instant. This situation is exactly like those we have considered earlier, like a Brownian particle or a noisy LR circuit.

Considering this random process giving rise to a fluctuational source, we want to compute the current autocorrelation function, which is a non-random description of the random process. The Fourier transform of it is proportional to the spectral density, our ultimate goal.

There are a few ways to attack the problem.

3.1 Boltzmann-Langevin approach

(pioneered by Shul'man, Kogan 1969)

- Use the regular BE to solve for the steady distribution of electrons under an applied field.
- About this non-equilibrium steady state, describe the fluctuations using the BE but now with Langevin sources added.
- Generally, the solution to the BE with this source can be written algebraically in terms of the Green's function of the BE, $G(1,2)$.
- With this form of the solution, compute the current autocorrelation function and use the correlation properties of the Langevin source. After some messy math, get an

expression for the current autocorrelation function in terms of and , the steady distribution.

This way works and is equivalent to the way that I will present (shown by Kogan, 1970). I will instead present the "method of moments" pioneered by Gantsevich, Gurevich, and Katilius because it is easier both conceptually and mathematically, and because they wrote the most accessible review paper on the topic [above authors, 1979]

3.2 Method of moments

The basic idea of this method is that we seek a kinetic-type equation for the ensemble average of the distribution autocorrelation function, , just like we have for the mean occupancy function .

I will review the BE material for the steady distribution to set the notation.

Consider a gas of charged particles (electrons) connected to a thermal bath of phonons. Without a field, the equilibrium distribution ensures that the mean rate of population transfer into a state by scattering is exactly balanced by that out of the state. Remember from the argument above there are instantaneous fluctuations in population owing to the variance in the population transfer rate. That produces current noise which in equilibrium we now know is Johnson-Nyquist noise.

When a field is applied, a redistribution of electrons in momentum space occurs because the electric field drives electrons to higher momentum states ( ).

That redistribution is governed by the BE. In this notation, neglecting ee collisions:

where is the time-dependent one-particle distribution function (bar indicates ensemble average).

Call the transition probability for a collision with the thermal bath that takes the electron from (occupied before collision) to (empty before collision). The ensemble

average of particle number in state is , and in state is . Therefore, the mean rate of particle number decrease in due to collisions is the difference in outflow and inflow:

Consider the non-degenerate situation. Then , so we have a linear collision matrix:

The transition probabilities have the property that the mean transition rate should vanish if we put in the equilibrium distribution . Therefore, we should have

We would like to solve this equation for the steady-state ensemble average distribution function , which satisfies the time-independent Boltzmann equation:

This distribution may have no resemblance to the equilibrium distribution. The mean energy per electron can be orders of magnitude larger than the equilibrium value depending on the strength of the field.

Let's suppose that we can solve this equation. Now, we want to consider the evolution of "small" deviations from this steady state. Let the time-dependent ensemble average of

occupancy be

The deviation term satisfies the BE also:

where is the same linearized operator we used for the steady problem. We denote as the relaxation operator. It consists of two parts: (1) streaming due to external field, , and (2) due to collisions.
We now see with this notation that the steady distribution satisfies

so that is an eigenfunction of with zero eigenvalue. Note that the distribution is normalized , the number of particles: .

The relaxation operator also determines the response from the non equilibrium steady state to a weak external perturbation. Suppose we apply an extra AC electric field: . The response of the deviations is:

We call the response operator.

3.3 Observables

If we know , we can calculate all experimental observables.
Steady current density :

Drift velocity :

Extra current from :

Using the BE obeyed by the deviation , we have

which uses the inverse response operator.
Therefore we find an expression for the AC differential conductivity:

The zero-frequency differential conductivity is

using the inverse relaxation operator.

We are now ready to consider fluctuations in the distribution function. Till now, we have considered mean values of the occupation numbers of one-particle states, the evolution of which is governed by the BE.

We now ask, what equation governs the evolution of the ensemble-averaged distribution auto-correlation function? This quantity is also called the time-displaced two-particle correlation function. It is defined as follows: we have fluctuations in the distribution about the mean:

We want the ensemble average of the product of fluctuations at two different time instants, :

As we've seen before, this quantity is a non-random characteristic of a random process, and its Fourier transform gives the spectral power density. We can compute a measurable quantity, the current density autocorrelation function, as

We want an equation for the time-displaced two-particle correlation function that we can solve, just like we solved for using the BE.
From very fundamental considerations, it can be derived that the appropriate equation is none other than:

Remarkably, obeys the same kinetic equation as the distribution function!
Some intuition: say at time a deviation in the distribution function is created due to the statistical nature of collisions. At a later time , the deviation in general would not be equal to zero even if, by coincidence, . If , the deviation at a later time consists of (1) what remains of the initial fluctuation and (2) any new fluctuations that have arisen after . In the thermodynamic limit , new fluctuations are independent of the one that occurred, e.g. at time . When we average over many realizations of a given fluctuation at time , we remove these new fluctuations. The reason is the new fluctuations are as likely to increase the population as decrease it since they are uncorrelated and hence average

to zero. With this type of average, becomes a smooth function of and describes the time evolution of a given initial deviation .

Now why does the Boltzmann equation describe the evolution of the initial deviation? Physically the origin of the fluctuation does not matter for the evolution - the evolution is the same whether the fluctuation was caused by a macroscopic perturbation or a statistical fluctuation (Onsager's 1931 regression hypothesis). So it is natural to think that the evolution of fluctuations should obey the BE. The difference is that is ensemble averaged over (1) realizations of a particular initial deviation and (2) over the set of initial deviations. The evolution is not affected by this latter averaging; the former average just gives the evolution of the mean which is precisely what the original BE describes (e.g. it describes the time evolution of the mean occupancy of quantum states). Therefore, we expect to follow the BE.

This is a reasonable argument; if you want a rigorous derivation, you can perform a quantum statistical treatment to obtain the result that also yields the BE itself as a bonus (GGK 1969).

3.4 One-time two particle correlation function

Since the equation given has a time derivative, we need an initial condition, e.g.

Let's first calculate the diagonal part of it :

For Fermi systems, the occupation of a quantum state can only be . So

For non-degenerate statistics ( ):

Now we need the off-diagonal terms of the one-time correlation function. Write the off-diagonal part as

The one-particle distribution function gives the mean occupancy of a state. This function describes the mean correlated occupancy of two different states. If the occupation numbers are completely uncorrelated (e.g. we have a grand canonical ensemble that allows for particles to enter and leave the system independently), .
However, in many electron systems in fact the particle number is fixed to . As Lax originally noted, this constraint leads to correlation. We get a multinomial distribution with a second moment given as

Therefore the constraint leads to correlations between occupancies of different states.
The final form of the initial condition for the two-time correlation function is:

3.5 Spectral density of distribution function fluctuations

With the initial condition and equation determined for , we can algebraically obtain the spectral density of distribution function fluctuations. It is the Fourier transform of the autocorrelation function:

For negative times, use the following identity and the stationarity of the process:

Then use the original governing equation, Fourier transformed, to get:

3.6 Relation to Langevin method

Rather than following the method of moments, we could have solved for the fluctuations themselves using the BE with a Langevin source term $y_p(t)$:

$$(\partial_t + I_p)\delta F_p(t) = y_p(t) \tag{2}$$

Then, the distribution function correlation function is

$$(\delta F_p \delta F_{p_1})_\omega = (-j\omega + I_p)^{-1}(j\omega + I_{p_1})^{-1}(y_p y_{p_1})_\omega \tag{3}$$

Therefore, to agree with the method of moments, we need the spectral density of the random force to be

$$(y_p y_{p_1})_\omega = (I_p + I_{p_1})\bar{F}_p \delta_{pp_1} \tag{4}$$

To obtain this expression you need to use Eq. 1.41 in Gantsevich 1979.
Undesirably, the external field E is in the expression for fluctuation source. It can be shown that these terms can be eliminated to get

$$(y_p y_{p_1})_\omega = \delta_{pp_1} \sum_k (W_k^p \bar{F}_p + W_p^k \bar{F}_k) - W_p^{p_1} \bar{F}_{p_1} - W_{p_1}^p \bar{F}_p \tag{5}$$

in terms of $\bar{F}$ and transition probabilities W only. This result is identical to that obtained in Shul'man, Kogan, 1969, who pursued a Green's function/Langevin approach.

3.7 Spectral density of current fluctuations

We now are ready to get the experimentally measurable and relevant quantity. The spectral density of spatially homogeneous current fluctuations is .

Substituting in our expression for , we get

For independent particles subject only to a constraint on total number , we use

to get

3.8 Equilibrium - Nyquist theorem

We can check that this expression reproduces the Nyquist theorem that relates current fluctuations to conductivity in equilibrium. In that case, the drift velocity , the frequency , and . The spectral density of current fluctuations is then:

Recalling our earlier expression for conductivity:

We see that:

So the Nyquist theorem holds!

3.9 Price-relation, fluctuation-diffusion relation

Wannier first derived that a diffusion coefficient in the non-equilibrium state could be defined as:

Price later derived (and it is also rigorously derived in Sec 2 of the Gantsevich review paper) this expression for the diffusion coefficient, and further showed that in the limit of , we can write

In other words, a relation exists between the non-equilibrium diffusion coefficient and the spectral density of current fluctuations! So although the original fluctuation-dissipation theorem linking spectral density and conductivity does not survive non-equilibrium, a fluctuation-diffusion relation still holds in the specified limit.

This result actually suggests an experimental method to measure noise temperature: impose a current on a sample and measure the diffusion coefficient by a time-of-flight method: impulsively heat electrons on one side of a sample and measure how long it takes them to reach the other side. We will discuss shortly.