Boltzmann-Green functions for nonequilibrium fluctuations in metallic systems

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I describe a method for calculating nonequilibrium fluctuations in degenerate conduction bands. The method uses Green-function propagators to solve the one-particle Boltzmann equation. In the equilibrium limit of the uniform electron gas, I confirm that the Nyquist noise theorem is recovered within this formalism. [S0163-1829(96)01132-0]

Solving the Boltzmann equation using Green functions is a simple and direct method for calculating nonequilibrium fluctuations of electrons in semiconductors. Their effectiveness in high-field noise modeling was demonstrated by Stanton and Wilkins[1–3] for classical electrons. The recent extension of the Boltzmann-Green functions to degenerate systems, within a relaxation-time approach,[4] shows their utility for calculating current noise in III-V heterojunctions[5] and their consequent importance for improved device optimization.

For Maxwell-Boltzmann statistics, there is no explicit distinction between the one-particle distribution and its fluctuation since they are strictly identical. What is different in my treatment of nonequilibrium Fermi-Dirac systems is the identification of the separate evolutions of these objects. In the classical limit they will of course coincide and the Stanton-Wilkins theory[1,2] is regained.

First, I describe a Boltzmann-Green-function formalism adaptable to metallic electron systems with realistic collision processes. Second, I verify an important property of the formalism in its low-field limit, the Nyquist theorem for degenerate conduction bands.[6] Last, I comment on the inclusion of many-body scattering processes within this approach.

For single-particle scattering situations, the semiclassical Boltzmann equation for the electron distribution function $f_\sigma(\mathbf{r},\mathbf{k};t)$ is

$$\frac{\partial f_\sigma}{\partial t}+\mathbf{v}_{\mathbf{k}\sigma}\cdot\frac{\partial f_\sigma}{\partial \mathbf{r}}-\frac{q\mathbf{E}(\mathbf{r},t)}{\hbar}\cdot\frac{\partial f_\sigma}{\partial \mathbf{k}} =\left[\frac{\partial f_\sigma}{\partial t}\right]_{\rm coll} =-\sum_{\mathbf{k}',\sigma'}[S_{\sigma'\sigma}(\mathbf{k}',\mathbf{k};\mathbf{E})f_\sigma(\mathbf{r},\mathbf{k},t) -S_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{E})f_{\sigma'}(\mathbf{r},\mathbf{k}',t)]. \quad (1)$$

The index σ labels the discrete subbands or valleys in a multilevel system, as well as the spin state. The field-dependent scattering rate S is assumed to satisfy microscopic reversibility, so that Eq. (1) holds equally for degenerate and classical populations.

To construct the time-dependent distribution and its fluctuation, one must begin by generating the steady-state form of f from the equilibrium solution $f^{\rm eq}_\sigma(\mathbf{r},\mathbf{k})$. For this we need Eq. (1) at equilibrium:

$$\mathbf{v}_{\mathbf{k}\sigma}\cdot\frac{\partial f^{\rm eq}_\sigma}{\partial \mathbf{r}}-\frac{q\mathbf{E}_0(\mathbf{r})}{\hbar}\cdot\frac{\partial f^{\rm eq}_\sigma}{\partial \mathbf{k}}=-\sum_{\mathbf{k}',\sigma'}[S_{\sigma'\sigma}(\mathbf{k}',\mathbf{k};\mathbf{E}_0)f^{\rm eq}_\sigma(\mathbf{r},\mathbf{k}) -S_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{E}_0)f^{\rm eq}_{\sigma'}(\mathbf{r},\mathbf{k}')] \equiv 0, \quad (2)$$

where the self-consistent internal field $\mathbf{E}_0(\mathbf{r})$ is defined in the absence of an external driving field. The quantities $f^{\rm eq}$ and $\mathbf{E}_0$ are linked by the usual constitutive relations, the first being Poisson's equation for the divergence of $\mathbf{E}_0(\mathbf{r})$ in terms of the density $n_0(\mathbf{r})=\langle f^{\rm eq}\rangle=\Omega^{-1}\Sigma_{\mathbf{k}',\sigma'}f^{\rm eq}_{\sigma'}(\mathbf{r},\mathbf{k}')$ (here Ω is the sample element's volume). The second relation is the form of the equilibrium function itself,

$$f^{\rm eq}_\sigma(\mathbf{r},\mathbf{k})=\frac{1}{1+\exp\{[E_\sigma(\mathbf{k})+V_0(\mathbf{r})-E_F]/k_BT\}}. \quad (3)$$

The gradient of the local potential V_0 is $q\mathbf{E}_0$ and E_F is the Fermi energy.

Define the difference function $g_\sigma(\mathbf{r},\mathbf{k})\equiv f_\sigma(\mathbf{r},\mathbf{k})-f^{\rm eq}_\sigma(\mathbf{r},\mathbf{k})$. From each side of Eq. (1) in the steady state, subtract its equilibrium counterpart. We obtain

$$\mathbf{v}_{\mathbf{k}\sigma}\cdot\frac{\partial g_\sigma}{\partial \mathbf{r}}-\frac{q\mathbf{E}(\mathbf{r})}{\hbar}\cdot\frac{\partial g_\sigma}{\partial \mathbf{k}}=\frac{q(\mathbf{E}-\mathbf{E}_0)}{\hbar}\cdot\frac{\partial f^{\rm eq}_\sigma}{\partial \mathbf{k}}+\left[\frac{\partial f_\sigma}{\partial t}\right]_{\rm coll}. \quad (4)$$

Recast $[\partial f/\partial t]_{\rm coll}$ in terms of g and $f^{\rm eq}$:

$$\left[\frac{\partial f_\sigma}{\partial t}\right]_{\rm coll}=-\sum_{\mathbf{k}',\sigma'}[S_{\sigma'\sigma}(\mathbf{k}',\mathbf{k};\mathbf{E})g_\sigma(\mathbf{r},\mathbf{k}) -S_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{E})g_{\sigma'}(\mathbf{r},\mathbf{k}')]-\sum_{\mathbf{k}',\sigma'}\{[S_{\sigma'\sigma}(\mathbf{k}',\mathbf{k};\mathbf{E}) -S_{\sigma'\sigma}(\mathbf{k}',\mathbf{k};\mathbf{E}_0)]f^{\rm eq}_\sigma(\mathbf{r},\mathbf{k})-[S_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{E}) -S_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{E}_0)]f^{\rm eq}_{\sigma'}(\mathbf{r},\mathbf{k}')\}. \quad (5)$$

Equations (4) and (5) define a standard integro-differential equation for g, with an inhomogeneous term directly dependent on $f^{\rm eq}$:

$$\sum_{\mathbf{k}',\sigma'}\Bigg\{\delta_{\mathbf{kk}'}\delta_{\sigma\sigma'}\Bigg[\mathbf{v}_{\mathbf{k}'\sigma'}\cdot\frac{\partial}{\partial\mathbf{r}}-\frac{q\mathbf{E}(\mathbf{r})}{\hbar}\cdot\frac{\partial}{\partial\mathbf{k}'}+\frac{1}{\tau_\sigma(\mathbf{k}';\mathbf{E})}\Bigg]-S_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{E})\Bigg\}g_{\sigma'}(\mathbf{r},\mathbf{k}')=\frac{q(\mathbf{E}-\mathbf{E}_0)}{\hbar}\cdot\frac{\partial}{\partial\mathbf{k}}f^{\mathrm{eq}}_\sigma(\mathbf{r},\mathbf{k})+\mathcal{C}_\sigma[f^{\mathrm{eq}}](\mathbf{r},\mathbf{k};\mathbf{E}),\tag{6}$$

where $\tau_\sigma^{-1}(\mathbf{k};\mathbf{E})=\Sigma_{\mathbf{k}',\sigma'}{}'S_{\sigma'\sigma}(\mathbf{k}',\mathbf{k};\mathbf{E})$ and the functional $\mathcal{C}[f^{\mathrm{eq}}]$ denotes the second sum of collision terms in Eq. (5).

The adiabatic response of the system about its nonequilibrium steady state is determined once the Boltzmann-Green function

$$G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{r})\equiv\frac{\delta g_\sigma(\mathbf{r},\mathbf{k})}{\delta f^{\mathrm{eq}}_{\sigma'}(\mathbf{r},\mathbf{k}')}\tag{7}$$

is known.[4] Since the difference solution g is generated explicitly from f^{eq}, the corresponding equation for G is easily derived by taking variations everywhere in Eq. (6). The propagator G determines the differential response of the nonequilibrium system to arbitrary perturbations of the underlying equilibrium state.

All of the steady-state fluctuation properties are definable in terms of G and the equilibrium background fluctuation Δf^{eq}. In particular, the steady-state fluctuation of the particle number is

$$\Delta f_\sigma(\mathbf{r},\mathbf{k})=\Delta f^{\mathrm{eq}}_\sigma(\mathbf{r},\mathbf{k})+\Delta g_\sigma(\mathbf{r},\mathbf{k})\equiv\Delta f^{\mathrm{eq}}_\sigma(\mathbf{r},\mathbf{k})+\sum_{\mathbf{k}',\sigma'}G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{r})\Delta f^{\mathrm{eq}}_{\sigma'}(\mathbf{r},\mathbf{k}'),\tag{8}$$

in which the equilibrium fluctuation Δf^{eq} is the density-density correlation function in the static long-wavelength limit,[7] up to a factor k_BT:

$$\Delta f^{\mathrm{eq}}_\sigma(\mathbf{r},\mathbf{k})\equiv k_BT\frac{\partial f^{\mathrm{eq}}_\sigma}{\partial E_F}=f^{\mathrm{eq}}_\sigma(1-f^{\mathrm{eq}}_\sigma).\tag{9}$$

Calculation of the time-dependent response requires the dynamical Boltzmann-Green function

$$\mathcal{R}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{r},t-t')\equiv\theta(t-t'^{+})\frac{\delta f_\sigma(\mathbf{r},\mathbf{k};t)}{\delta f_{\sigma'}(\mathbf{r},\mathbf{k}';t')},\tag{10}$$

with initial value $\mathcal{R}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{r},0^+)=\delta_{\mathbf{kk}'}\delta_{\sigma\sigma'}$. In the frequency domain, its Fourier transform $\hat{\mathcal{R}}$ satisfies the following form of Eq. (1):

$$\sum_{\mathbf{k}'',\sigma''}\Bigg\{\delta_{\mathbf{kk}''}\delta_{\sigma\sigma''}\Bigg[\mathbf{v}_{\mathbf{k}''\sigma}\cdot\frac{\partial}{\partial\mathbf{r}}-\frac{q\mathbf{E}(\mathbf{r})}{\hbar}\cdot\frac{\partial}{\partial\mathbf{k}''}+\frac{1}{\tau_\sigma(\mathbf{k}'';\mathbf{E})}-i\omega\Bigg]-S_{\sigma\sigma''}(\mathbf{k},\mathbf{k}'';\mathbf{E})\Bigg\}\hat{\mathcal{R}}_{\sigma''\sigma'}(\mathbf{k}'',\mathbf{k}';\mathbf{r},\omega)=\delta_{\mathbf{kk}'}\delta_{\sigma\sigma'}.\tag{11}$$

All of the dynamical fluctuation properties are definable in terms of $\hat{\mathcal{R}}$ and the nonequilibrium background fluctuation Δf. In particular, the dynamical velocity autocorrelation function is

$$\langle\langle\mathbf{v}\mathbf{v}'\Delta\hat{f}(\mathbf{r};\omega)\rangle\rangle'\equiv\frac{1}{\Omega}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'}\mathbf{v}_{\mathbf{k}\sigma}\hat{\mathcal{R}}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\mathbf{r},\omega)\mathbf{v}_{\mathbf{k}'\sigma'}\Delta f_{\sigma'}(\mathbf{r},\mathbf{k}').\tag{12}$$

Physically, Eq. (12) states that a random excursion of the distribution function out of the nonequilibrium steady state will undergo a dynamical evolution governed by Eq. (11), carrying with it the temporal correlations.[8]

I now show that the Nyquist theorem for degenerate, multilevel conduction bands holds within the Boltzmann-Green-function prescription. (Reference 3, Appendix 2A, details the proof for classical Boltzmann-Green functions.) Consider a homogeneous electron gas, of density n_s. The equilibrium field $\mathbf{E}_0$ is zero. Let the driving field be $\mathbf{E}=\mathcal{E}\hat{\mathbf{x}}$. Assuming that the field dependence of the scattering rate vanishes faster than $\mathcal{E}$, the functional $\mathcal{C}[f^{\mathrm{eq}}]$ can be dropped from Eq. (6).

The form of the current density $J=-q\langle v_xg\rangle=-q/\Omega\Sigma_{\mathbf{k},\sigma}(v_x)_{\mathbf{k}\sigma}g_\sigma(\mathbf{k})$ yields an expression for the differential mobility μ:

$$\mu(\mathcal{E})=\frac{1}{qn_s}\frac{\partial J}{\partial\mathcal{E}}=-\frac{1}{n_s\Omega}\sum_{\mathbf{k},\sigma}(v_x)_{\mathbf{k}\sigma}\frac{\partial g_\sigma}{\partial\mathcal{E}}(\mathbf{k}).\tag{13}$$

The derivative $\partial g_\sigma/\partial\mathcal{E}$ satisfies an equation obtained from Eq. (6) by differentiating each side:

$$\sum_{\mathbf{k}',\sigma'}\Bigg\{\delta_{\mathbf{kk}'}\delta_{\sigma\sigma'}\Bigg[-\frac{q\mathcal{E}}{\hbar}\frac{\partial}{\partial k'_x}+\frac{1}{\tau_\sigma(k')}\Bigg]-S_{\sigma\sigma'}(\mathbf{k},\mathbf{k}')\Bigg\}\frac{\partial g_{\sigma'}}{\partial\mathcal{E}}(\mathbf{k}')=\frac{q}{\hbar}\frac{\partial}{\partial k_x}(f^{\mathrm{eq}}_\sigma+g_\sigma).\tag{14}$$

On the other hand, the difference propagator G obeys the equation

$$\sum_{\mathbf{k}'',\sigma''}\Bigg\{\delta_{\mathbf{kk}''}\delta_{\sigma\sigma''}\Bigg[-\frac{q\mathcal{E}}{\hbar}\frac{\partial}{\partial k''_x}+\frac{1}{\tau_\sigma(k'')}\Bigg]-S_{\sigma\sigma''}(\mathbf{k},\mathbf{k}'')\Bigg\}G_{\sigma''\sigma'}(\mathbf{k}'',\mathbf{k}')=\delta_{\mathbf{kk}'}\delta_{\sigma\sigma'}\frac{q\mathcal{E}}{\hbar}\frac{\partial}{\partial k'_x}.\tag{15}$$

A comparison of Eqs. (14) and (15) results in

$$\frac{\partial g_\sigma}{\partial\mathcal{E}}(\mathbf{k})=\frac{1}{\mathcal{E}}\Bigg(g_\sigma(\mathbf{k})+\sum_{\mathbf{k}',\sigma'}G_{\sigma\sigma'}(\mathbf{k},\mathbf{k}')g_{\sigma'}(\mathbf{k}')\Bigg),\tag{16}$$

where $\Sigma Gg\sim\mathcal{E}^2$ in the low-field limit.

Now convolve the right-hand expression in the relation

$$\frac{\partial f^{\mathrm{eq}}_\sigma}{\partial k_x}=-\frac{\hbar}{k_BT}(v_x)_{\mathbf{k}\sigma}\Delta f^{\mathrm{eq}}_\sigma(k),\tag{17}$$

with Eq. (11) in the static limit $\omega\to0$. The resulting equation is numerically equivalent to Eq. (6). Therefore

$$\frac{g_\sigma(\mathbf{k})}{\mathcal{E}}=-\frac{q}{k_BT}\sum_{\mathbf{k}',\sigma'}\hat{\mathcal{R}}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}';\omega=0)(v_x)_{\mathbf{k}'\sigma'}\Delta f^{\mathrm{eq}}_{\sigma'}(k').\tag{18}$$

Combining Eqs. (13), (16), and (18) when $\mathcal{E}\rightarrow 0$, I conclude that

$$\mu = \frac{q}{n_s k_B T}\langle\langle v_x v_x' \Delta \hat{f}(\omega=0)\rangle\rangle', \tag{19}$$

which is the Einstein relation when the velocity autocorrelation function is expressed in terms of the diffusion constant[9] $\hat{D}_{xx} \equiv n_s^{-1}\langle\langle v_x v_x' \Delta \hat{f}\rangle\rangle'$.

The Nyquist theorem follows. For definiteness, take a two-dimensional electron gas with sample area $\Omega = L_x L_y$. Given the total current I and applied voltage V, then $\partial J/\partial\mathcal{E} = (I/L_y)/(V/L_x) = L_x^2/(\Omega R)$, where R is the macroscopic sample resistance. The current-current spectral density for $n_s\Omega$ carriers is given by[9] $S^{II}(\omega,\mathcal{E}) \equiv 4 n_s \Omega[(q/L_x)^2 \hat{D}_{xx}(\omega,\mathcal{E})]$. Thus Eq. (19) is equivalent to

$$S^{II}(0,0) = 4 k_B T \frac{1}{R}, \tag{20}$$

confirming that the Nyquist result is contained within the fluctuation structure of this framework.

I close with some remarks on many-body effects. The Boltzmann-Green function approach obviously gains in scope with the inclusion of multiparticle scattering, be it electron-electron, electron-phonon, or other. The cost of this is a collision term nonlinear in g and linearized equations for G and $\mathcal{R}$, which now depend on g explicitly.[10]

At low densities and high temperatures, the present formalism describes a weakly coupled classical plasma, as in the theory of Stanton and Wilkins.[1–3] In the strongly degenerate limit of high density and low temperature, the dominance of E_F over $k_B T$ means that collective plasma dynamics are frozen out and Born-Oppenheimer mode decoupling is valid.[7] In this case $\Delta f^{\rm eq}$ becomes, to a very good approximation, the density-density correlation function screened with a static local-field correction.[11,12]

In the intermediate regime, the tools of choice for transport problems are quantum-kinetic equations.[13,14] For high fields, however, truly practical calculations, especially of noise, are rare. Simplified quantum-kinetic formulations with Boltzmann-like structures have been set up to deal with specific problems[10,15,16] and it may be possible to extend them. The conceptual similarity between nonequilibrium Boltzmann-Green functions and the particle-hole vertex propagators of many-body theory[7] encourages further investigation.

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