Classical Langevin equations for the free electron

gas and blackbody radiation

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Abstract. Among others, Uhling and Uhlenbeck, Kaniadakis and Quarati, and

Kadanoff have suggested to describe the evolution of quantum systems exhibiting

Fermi-Dirac and Bose-Einstein statistics by means of classical but nonlinear evolution

equations for density measures such as generalized Boltzmann equations and nonlinear

Fokker-Planck equations. We use this approach in order to derive classical Langevin

equations for quantum systems and apply the Langevin equations thus obtained to two

fundamental quantum systems, namely, the free electron gas and blackbody radiation.

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1. Introduction

In line with early studies by *Uhling* and *Uhlenbeck* [1, 2], several authors have been suggested to describe the evolution of quantum systems exhibiting Fermi-Dirac and Bose-Einstein statistics by means of Fokker-Planck equations that are nonlinear with respect to density measures [3, 4, 5, 6, 7, 8, 9]. The nonlinearities reflect the quantum mechanical constraints on Fermi and Bose systems. So far, however, this approach to quantum systems is incomplete with respect to two issues. First, the approach ignores the degeneracy of energy levels. Second, the approach has not been applied to quantum mechanical benchmark systems such as the free electron gas and blackbody radiation. In this letter, we address both issues within the framework of Langevin equations related to nonlinear Fokker-Planck equations of quantum systems.

2. Generalized Fokker-Planck and Langevin equations

2.1. Free energy principle

Let us consider a system with N energy levels $\epsilon_1, \ldots, \epsilon_N$. Let ρ_i denote the mean occupation number of the energy level i. Finally, let $g_i > 0$ describe the number of different quantum states that belong to the same energy level ϵ_i , that is, the degeneration of the energy level i. Then the quantum entropy for Fermi and Bose particles reads [10]

$$^{\text{FD,BE}}S(\rho_1,\ldots,\rho_N) = -\sum_{i=1}^N \rho_i \ln \rho_i + \sum_{i=1}^N g_i \ln g_i \mp \sum_{i=1}^N (g_i \mp \rho_i) \ln(g_i \mp \rho_i) . (1)$$

Note that here and in what follows the upper sign refers to Fermi systems, while the lower sign refers to Bose systems. In the case of Fermi systems we require that the inequality $\rho_i < g_i$ holds for temperatures T > 0. For T = 0 we have $\rho_i = g_i$ up to the Fermi energy ϵ_F and $\rho_i = 0$ for energy states i with $\epsilon_i > \epsilon_F$. Studying systems with continuous energy levels $\epsilon \in \Omega = [0, \infty)$, we replace g_i by a function $g(\epsilon) \geq 0$. The expression $g(\epsilon)$ describes the number of states in an energy range between ϵ and $\epsilon + d\epsilon$. That is, $g(\epsilon)$ describes the density of states with respect to the energy scale ϵ

[11]. Using $g(\epsilon)$, we modify Eq. (1) in order to become

$$FD,BES[\rho] = -\int_{\Omega} \rho(\epsilon) \ln \rho(\epsilon) d\epsilon + \int_{\Omega} g(\epsilon) \ln g(\epsilon) d\epsilon$$

$$\mp \int_{\Omega} [g(\epsilon) \mp \rho(\epsilon)] \ln[g(\epsilon) \mp \rho(\epsilon)] d\epsilon . \tag{2}$$

Here, $\rho(\epsilon)$ describes the mean occupation number density on a continuous energy scale. In the case of Fermi systems the constraint $\rho(\epsilon) < g(\epsilon)$ for T > 0 holds. Now, let us consider the free energy

$$F[\rho] = U[\rho] - T^{\text{FD,BE}}S[\rho] \tag{3}$$

with

$$U[\rho] = \int_{\Omega} \epsilon \rho(\epsilon) \, \mathrm{d}\epsilon \ . \tag{4}$$

In order to derive stationary distributions $\rho_{\rm st}$ from the free energy principle $\delta F/\delta \rho = \mu$, we need to compute the variational derivatives of U and $^{\rm FD,BE}S$. They read

$$\frac{\delta U}{\delta \rho} = \epsilon \tag{5}$$

and

$$\frac{\delta}{\delta \rho}^{\text{FD,BE}} S = -\ln\left(\frac{\rho}{g \mp \rho}\right) . \tag{6}$$

From $\delta F/\delta \rho = \mu$ and Eqs. (3), (5), (6), we obtain the Fermi-Dirac and Bose-Einstein distributions for quantum systems with degenerated energy levels:

$$\rho_{\rm st}(\epsilon) = \frac{g(\epsilon)}{\exp\{(\epsilon - \mu)/T\} \pm 1} \ . \tag{7}$$

2.2. Fokker-Planck equation

In line with recent studies on nonlinear Fokker-Planck equations, we assume that $\rho(\epsilon, t)$ satisfies the free energy Fokker-Planck equation

$$\frac{\partial}{\partial t}\rho(\epsilon,t) = \frac{\partial}{\partial \epsilon}\rho \frac{\partial}{\partial \epsilon} \frac{\delta F}{\delta \rho} , \qquad (8)$$

see [3, 4, 5, 6, 7, 9, 12, 13, 14, 15, 16, 17] in general and [8] in particular. The benefits of Fokker-Planck equations of the form (8) are at least twofold. First, equilibrium distributions obtained from $\delta F/\delta \rho = \mu$ correspond to stationary solutions of Eq. (8).

Since for solutions of Eq. (8) we have $dF/dt \leq 0$ (see Eq. (9) below), (stable) stationary solutions correspond to free energy minima. This is tantamount to say that in the stationary case we deal with maximum entropy distributions of canonical ensembles. Second, transient solutions of Eq. (8) converge to stationary ones in the long time limit provided that entropy measures are concave [5, 8, 9, 13]. The reason for this is that for transient solutions of Eq. (8) the functional F satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}F[\rho] = -\int_{\Omega} \rho \left[\frac{\partial}{\partial \epsilon} \frac{\delta F}{\delta \rho} \right]^2 \, \mathrm{d}\epsilon \le 0 \ . \tag{9}$$

By definition of the functional $F[\rho]$, we have $\mathrm{d}\rho/\mathrm{d}t=0\Rightarrow\mathrm{d}F/\mathrm{d}t=0$ and from Eq. (9) it is clear that $\mathrm{d}F/\mathrm{d}t=0\Rightarrow\delta F/\delta\rho=\mathrm{const}$, which implies that $\mathrm{d}F/\mathrm{d}t=0\Rightarrow\mathrm{d}\rho/\mathrm{d}t=0$. Furthermore, let us write S as $S[\rho]=\int_\Omega s(\rho,g)\,\mathrm{d}\epsilon$ with $g=g(\epsilon)$. If $\partial^2 s/\partial\rho^2\leq 0$ for all ϵ , then s satisfies the concavity inequality $s(\rho,g)\leq s(\rho',g)+(\rho-\rho')\partial s/\partial\rho'$ for all ϵ and S is a concave functional. From the concavity of S, in turn, it follows that $F[\rho]\geq F[\rho_{\mathrm{st}}]$ [18, 19]. In fact, evaluating Eq. (2) we find that $\partial^2 s/\partial\rho^2=-g/[\rho(g\mp\rho)]$. In particular, for fermions we have $\partial^2 s/\partial\rho^2=-g/[\rho(g-\rho)]$. Due to the constraint $\rho(\epsilon,\cdot)< g(\epsilon)$, we obtain $\partial^2 s/\partial\rho^2\leq 0$. For bosons we get $\partial^2 s/\partial\rho^2=-g/[\rho(g+\rho)]\leq 0$. Therefore, S is concave and F is bounded from below for arbitrary density of state functions g satisfying $g(\epsilon)\geq 0$. In sum, we have shown that the relations

$$\frac{\mathrm{d}}{\mathrm{d}t}F[\rho] \le 0$$
, $\frac{\mathrm{d}}{\mathrm{d}t}F[\rho] = 0 \Leftrightarrow \frac{\partial}{\partial t}\rho = 0$, F bounded from below (10)

hold. From these relations we read off that F is a Lyapunov functional and conclude that transient solutions converge to stationary ones in the limit $t \to \infty$.

2.3. Langevin equation

Substituting Eqs. (3), (5) and (6) into Eq. (8), we obtain

$$\frac{\partial}{\partial t}\rho(\epsilon,t) = \frac{\partial\rho}{\partial\epsilon} + \underbrace{T\frac{\partial}{\partial\epsilon}\rho\frac{\partial}{\partial\epsilon}\frac{\rho}{g\mp\rho}}_{V}.$$
(11)

Let us evaluate the expression Y. First, we note that

$$\rho \frac{\partial}{\partial \epsilon} \frac{\rho}{g \mp \rho} = \pm \frac{\mathrm{d}g}{\mathrm{d}\epsilon} \left[1 + \ln(g \mp \rho) \right] \mp \frac{\mathrm{d}}{\mathrm{d}\epsilon} \left[g \ln(g \mp \rho) \right] . \tag{12}$$

Then, Eq. (11) becomes

$$\frac{\partial}{\partial t}\rho(\epsilon,t) = \frac{\partial\rho}{\partial\epsilon} \pm T\frac{\partial}{\partial\epsilon} \left\{ \frac{\mathrm{d}g}{\mathrm{d}\epsilon} \left[1 + \ln(g \mp \rho) \right] \right\} \mp T\frac{\partial^2}{\partial\epsilon^2} g \ln(g \mp \rho) \ . \tag{13}$$

Eq. (13) is well-defined in the limit $\rho \to 0$ because Eq. (13) is homogenous with respect to ρ . That is, $\rho = 0$ is a solution of Eq. (13). In order to obtain a semi-positive definite diffusion coefficient, we write the term $g \ln(g \mp \rho)$ in Eq. (13) as $g \ln(g \mp \rho) = g \ln(1 \mp \rho/g) + g \ln(g)$, which gives us

$$\frac{\partial}{\partial t}\rho(\epsilon,t) = -\frac{\partial}{\partial \epsilon} \left\{ \left[-1 \mp \frac{T}{\rho} \frac{\mathrm{d}g}{\mathrm{d}\epsilon} \ln\left(1 \mp \frac{\rho}{g}\right) \right] \rho \right\} \mp T \frac{\partial^2}{\partial \epsilon^2} g \ln\left(1 \mp \frac{\rho}{g}\right) . \tag{14}$$

Note that we have a reflective boundary at $\epsilon = 0$ with $\rho(0, t) = 0$. The drift and diffusion coefficients read

$$d_1(\epsilon, \rho) = -1 \mp \frac{T}{\rho} \frac{\mathrm{d}g(\epsilon)}{\mathrm{d}\epsilon} \ln \left(1 \mp \frac{\rho}{g(\epsilon)} \right) , \qquad (15)$$

$$d_2(\epsilon, \rho) = \mp T \frac{g(\epsilon)}{\rho} \ln \left(1 \mp \frac{\rho}{g(\epsilon)} \right)$$
 (16)

such that Eq. (14) can be written as

$$\frac{\partial}{\partial t}\rho(\epsilon,t) = -\frac{\partial}{\partial \epsilon}d_1(\epsilon,\rho)\rho + \frac{\partial^2}{\partial \epsilon^2}d_2(\epsilon,\rho)\rho . \tag{17}$$

The diffusion coefficient d_2 is positive definite which can be seen if we distinguish explictly between Fermi and Bose systems. For Fermi systems we obtain $d_2 = Tg \ln(1/(1-\rho/g)) > 0$ for $0 < \rho(\epsilon) < g(\epsilon)$. For Bose systems we have $d_2 = Tg \ln(1+\rho/g)) > 0$ for $\rho(\epsilon) > 0$. By similar reasonings, we see that the drift term is composed of an attractive and repulsive part: $d_1 = d_1(-) + d_1(+)$. The attractive part is given by $d_1(-) = -1$ and drives particles to states of the ground state energy equal to zero. The repulsive part reads $d_1(+) = \mp T\rho^{-1}\mathrm{d}g/\mathrm{d}\epsilon \ln(1 \mp \rho/g) > 0$ and drives the quantum particles away from the ground state energy provided that the density of energy states increases with the energy (i.e., we have $\mathrm{d}g/\mathrm{d}\epsilon > 0$). Due to the interplay of these two forces, stable stationary distributions can be established. If the occupation number density ρ is normalized to M_0 with $M_0 = \int_{\Omega} \rho(\epsilon) \,\mathrm{d}\epsilon$, we can substitute $P(\epsilon,t;u) = \rho(\epsilon,t)/M_0$ into Eq. (14) and thus obtain a nonlinear Fokker-Planck equation

for the probability density P. We proceed now under the hypothesis that the Fokker-Planck equation thus obtained is a strongly nonlinear Fokker-Planck equation such that solutions of the nonlinear Fokker-Planck equation can alternatively be computed from an appropriately defined Langevin equation [20, 21]. This self-consistent Ito-Langevin equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\epsilon_{L}(t) = -1 \mp \frac{T}{M_{0} \left\langle \delta(\epsilon - \epsilon_{L}(t)) \right\rangle} \frac{\mathrm{d}g(\epsilon)}{\mathrm{d}\epsilon} \ln \left(1 \mp \frac{M_{0} \left\langle \delta(\epsilon - \epsilon_{L}(t)) \right\rangle}{g(\epsilon)} \right) \Big|_{\epsilon = \epsilon_{L}(t)} + \sqrt{\mp T \frac{g(\epsilon)}{M_{0} \left\langle \delta(\epsilon - \epsilon_{L}(t)) \right\rangle} \ln \left(1 \mp \frac{M_{0} \left\langle \delta(\epsilon - \epsilon_{L}(t)) \right\rangle}{g(\epsilon)} \right)} \Big|_{\epsilon = \epsilon_{L}(t)} \Gamma(t) \tag{18}$$

and is related to ρ by means of the ensemble average $\rho(\epsilon,t) = M_0 \langle \delta(\epsilon - \epsilon_L(t)) \rangle$. Let us apply now the Ito-Langevin equation (18) to describe the quantum statistics of electron gases and blackbody radiation.

2.4. Free electron gas

The electrons of the conduction band of metals can be regarded as a gas of fermions that are distributed over a continuous energy scale. In what follows we consider a free electron gas for which the density of states is given by $g(\epsilon) = a\sqrt{\epsilon}$ with a > 0 [11]. Consequently, we have $dg/d\epsilon = a/(2\sqrt{\epsilon})$ and the Fermi Fokker-Planck equation (14) (upper sign) becomes

$$\frac{\partial}{\partial t}\rho(\epsilon,t) = -\frac{\partial}{\partial \epsilon} \left\{ \left[-1 - \frac{aT}{2\sqrt{\epsilon}\rho} \ln\left(1 - \frac{\rho}{a\sqrt{\epsilon}}\right) \right] \rho \right\}
- aT \frac{\partial^2}{\partial \epsilon^2} \sqrt{\epsilon} \ln\left(1 - \frac{\rho}{a\sqrt{\epsilon}}\right) .$$
(19)

The corresponding Ito-Langevin equation (18) reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\epsilon_{L}(t) = -1 - \frac{aT}{2M_{0}\sqrt{\epsilon}\left\langle\delta(\epsilon - \epsilon_{L}(t))\right\rangle} \ln\left(1 - \frac{M_{0}\left\langle\delta(\epsilon - \epsilon_{L}(t))\right\rangle}{a\sqrt{\epsilon}}\right)\Big|_{\epsilon = \epsilon_{L}(t)} + \sqrt{-T\frac{a\sqrt{\epsilon}}{M_{0}\left\langle\delta(\epsilon - \epsilon_{L}(t))\right\rangle} \ln\left(1 - \frac{M_{0}\left\langle\delta(\epsilon - \epsilon_{L}(t))\right\rangle}{a\sqrt{\epsilon}}\right)}\Big|_{\epsilon = \epsilon_{L}(t)} \Gamma(t) . \tag{20}$$

Eq. (20) is subjected to the constraint $\rho(\epsilon) < a\sqrt{\epsilon}$ for T > 0. In the case of the free electron gas the stationary solution (7) reads

$$\rho_{\rm st}(\epsilon) = \frac{a\sqrt{\epsilon}}{\exp\{(\epsilon - \mu)/T\} + 1} \tag{21}$$

Insert Figure 1 and 2 about here

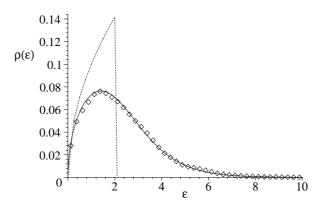


Figure 1. Stationary solution of the Fermi Fokker-Planck equation (19). Solid line: analytical result (21). Diamonds: numerical results obtained by solving the Ito-Langevin equation (20). Dashed line: stationary solution in the limiting case $T \to 0$. Parameters: $\mu = \epsilon_F = 2$, T = 1.0, a = 0.1.

for T>0, where μ corresponds to the Fermi energy ϵ_F . In the limit $T\to 0$ we obtain $\rho_{\rm st}(\epsilon)=a\sqrt{\epsilon}$ for $\epsilon\leq\mu=\epsilon_F$ and $\rho_{\rm st}(\epsilon)=0$ for $\epsilon>\mu=\epsilon_F$. In order to simulate the electron gas by means of the Ito-Langevin equation (20) for a particular Fermi energy ϵ_F , we first compute M_0 by means of $M_0=\int_\Omega \rho_{\rm st}(\epsilon)\,\mathrm{d}\epsilon$ and substitute the result into Eq. (20). We then solve Eq. (20) by means of an Euler forward scheme that is described in detail in [22]. Figure 1 shows the stationary distribution of the free electron gas as obtained from Eq. (21) and from a simulation of the Ito-Langevin equation (20). The dashed line describes the Fermi distribution at T=0. In order to solve the Ito-Langevin equation (20) numerically it is important to choose an initial distribution that satisfies the constrain $\rho(\epsilon) < g(\epsilon) = a\sqrt{\epsilon}$, see Fig. 2.

2.5. Blackbody radiation

The electromagnetic radiation in a black body cavity exhibits a frequency distribution $\rho(\nu)$ given by a Bose-Einstein statistics [11]. Let us describe the radiation field as a photon gas composed of photons with frequencies ν and energies $\epsilon = h\nu$, where h is

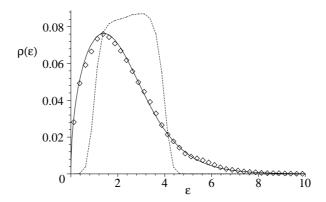


Figure 2. Stationary solution as in Fig. 1 (solid line and diamonds). In addition, the initial distribution that was used to solve the Ito-Langevin equation numerically is shown. The initial distribution corresponds approximately to a uniform distribution in the range between $\epsilon = 1$ and $\epsilon = 4$ and satisfies the constraint $\rho(\epsilon) < g(\epsilon)$.

Planck's constant. For the sake of conveniency, we put h = 1 such that $\epsilon = \nu$. The density of states of the photon gas is given by $g(\nu) = a\nu^2$ with a > 0, which implies $dg/d\nu = 2a\nu$. Consequently, the Bose Fokker-Planck equation (14) (lower sign) for the photon gas is given by

$$\frac{\partial}{\partial t}\rho(\nu,t) = -\frac{\partial}{\partial \nu} \left\{ \left[-1 + \frac{2aT\nu}{\rho} \ln\left(1 + \frac{\rho}{a\nu^2}\right) \right] \rho \right\} + aT \frac{\partial^2}{\partial \nu^2} \nu^2 \ln\left(1 + \frac{\rho}{a\nu^2}\right)$$
(22)

and the Ito-Langevin equation (18) reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\nu_{L}(t) = -1 + \frac{2aT\nu}{M_{0}\left\langle\delta(\nu - \nu_{L}(t))\right\rangle} \ln\left(1 + \frac{M_{0}\left\langle\delta(\nu - \nu_{L}(t))\right\rangle}{a\nu^{2}}\right) \Big|_{\nu = \nu_{L}(t)} + \sqrt{\frac{a\nu^{2}T}{M_{0}\left\langle\delta(\nu - \nu_{L}(t))\right\rangle} \ln\left(1 + \frac{M_{0}\left\langle\delta(\nu - \nu_{L}(t))\right\rangle}{a\nu^{2}}\right)} \Big|_{\nu = \nu_{L}(t)} \Gamma(t) . \tag{23}$$

Since the chemical potential μ of photons equals zero, the stationary solution (7) reads

$$\rho_{\rm st}(\nu) = \frac{a\nu^2}{\exp\{\nu/T\} - 1} \ . \tag{24}$$

The spectral energy density $u(\nu)$ of a cavity with volume V=1 is defined by $u(\nu)=\nu\rho_{\rm st}(\nu)$ [23]. Using Eq. (24), we obtain Planck's radiation formula

$$u(\nu) = \frac{a\nu^3}{\exp\{\nu/T\} - 1} \ . \tag{25}$$

Insert Figure 3 and 4 about here

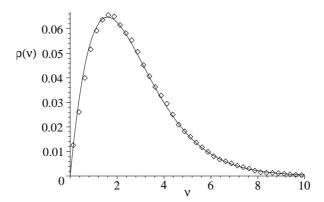


Figure 3. Stationary solution of the Bose Fokker-Planck equation (22). Solid line: analytical result (24). Diamonds: numerical results obtained by solving the Ito-Langevin equation (23). Parameters: T = 1.0, a = 0.1.

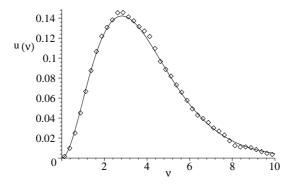


Figure 4. Illustration of Planck's radiation formula. Planck's formula as obtained from Eq. (25) (solid line) and as obtained by solving numerically the Ito-Langevin equation (23) (diamonds). Parameters as in Fig. 3.

From Eq. (24) and $\nu \in \Omega = [0, \infty)$ it follows that the total mass M_0 of the photon gas for a particular temperature T is given by $M_0 = \int_0^\infty \rho_{\rm st}(\nu) \, \mathrm{d}\nu$. If we substitute this M_0 -value into Eq. (23), we obtain a closed description of the stochastic evolution of the photon frequencies ν . In particular, $\rho(\nu,t)$ and $u(\nu)$ can be computed from $\rho(\nu,t) = M_0 \langle \delta(\nu - \nu_L(t)) \rangle$ and $u(\nu) = M_0 \nu \langle \delta(\nu - \nu_L(t)) \rangle_{\rm st}$, see Figs. 3 and 4.

3. Conclusions

We have studied a classical Fokker-Planck equation describing both the relaxation of Fermi and Bose systems to stationary states and the quantum statistics in these stationary states. In addition, the corresponding Langevin equation describing the motion of single quantum particles has been derived. In contrast to several previous studies, we included in our considerations the density of quantum states. In doing so, we have been able to apply our approach to the free electron gas of metal electrons and the blackbody radiation. Finally, we would like to point out that the results obtained here might be applied to classical systems that behave like Fermi systems. For example, it has been suggested that vortices of turbulent flows and grains of granular matter can be described by means of Fermi-Dirac statistics (see, e.g., [9, 24]).

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