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# Nonequilibrium quantum stochastic thermodynamics for bosons and fermions

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**Abstract** We use a canonical quantization procedure to obtain the quantum Fokker–Planck equation for a system of interacting particles, which can be either bosons or fermions. Based on this equation, we develop a quantum stochastic thermodynamics of equilibrium and nonequilibrium systems. The approach is applied to a system in contact with two reservoirs of heat and particles from which we determine the entropy production rate, as well as the heat and particle fluxes. When applied to noninteracting systems, we obtain the usual expression for the mean occupation number for bosons and for fermions.

## 1 Introduction

The distinguishing feature of stochastic thermodynamics [1–9] is the use of a dynamics that is stochastic in nature. If the space of states is continuous, this dynamics is well described by the Fokker–Planck (FP) equation [10, 11] which governs the time evolution of the probability density. When applied to a system of interacting particles, the FP equation is capable of describing the states out of thermodynamic equilibrium as well as the thermodynamic equilibrium [1]. If the system to be studied is a quantum system, we need a quantum version of the FP to represent the stochastic dynamics. One way of reaching the quantum version is by means of canonical quantization [12].

The canonical quantization procedure that we use here led us to a quantum FP equation which can be understood as the quantum Liouville plus a term associated to quantum dissipation. Other approaches to a quantum stochastic equation with this structure have been devised [13–24] such as that proposed by Lindblad [13] and that by Caldeira and Leggett [19, 20].

We set up a quantum FP equation using a representation in terms of the creation and annihilation operators that is appropriate for a systems of bosons and fermions. We start with a Langevin equation written in terms of complex conjugate dynamic variables from which we find the associated FP equation. This equation is written in a canonical form from which we get the quantum FP equation by a canonical quantization. The resulting equation for a system with one degree of freedom has the following structure

$$i\hbar\frac{\partial\rho}{\partial t} = [H,\rho] - [a, J^\dagger] - [a^\dagger, J], \qquad (1)$$

where $\rho$ is the density operator, $H$ is the Hamiltonian, $a$ and $a^\dagger$ are the annihilation and creation operators, and $J$ is the current associated to the density operator. The appropriate form of $J$ is found by imposing the condition that in thermodynamic equilibrium, the system is described by the Gibbs state. This condition guarantees that the usual expressions for the mean occupation number of bosons and fermions are obtained for a system of non-interacting particles.

After setting up the quantum FP equation for one degree of freedom, we generalize the equation for several degrees of freedom, which is appropriate for a system of interacting particles. Based on this quantum equation we develop the quantum stochastic thermodynamic for boson and fermion systems in equilibrium and out of equilibrium. This includes the definition of the rate of entropy production and of the heat and particle fluxes.

We apply the formalism developed here to the case of a system in contact with two reservoirs of heat and of particles at distinct temperatures and chemical potentials. We determine the heat and particle fluxes through the system at the stationary state as well as the rate of the entropy production. The corresponding Onsager coefficients are also determined.

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## 2 Complex conjugate variables

The equations of motion associated to a classical system with one degree of freedom under the action of a conservative force are given by

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial x}, \tag{2}$$

where $q$ and $p$ are the canonical variables and $H$ is the Hamiltonian, which is a real function.

Instead of the conjugate variables $q$ and $p$, we may use another pair of variables that are obtained by a canonical transformation. Here we use a peculiar canonical pair of variables, denoted by $a$ and $a^*$, that are complex conjugates of one another [25]. They are obtained from the real $q$ and $p$ by the transformation

$$a = c_1 q + ic_2 p, \tag{3}$$

where $c_1$ and $c_2$ are real, and $c_1 c_2 = 1/2$. Using this transformation, the two equations of motion are reduced to just one complex equation of motion

$$i\frac{da}{dt} = \frac{\partial H}{\partial a^*}, \tag{4}$$

where the Hamiltonian $H$ is a real function of $a$ and $a^*$.

A Langevin equation of motion is set up by adding a dissipation and a fluctuation term to Eq. (4),

$$i\frac{da}{dt} = \frac{\partial H}{\partial a^*} - i\gamma g + i\zeta, \tag{5}$$

where the term $\gamma g$ represents the dissipation, $\gamma$ being its strength, and $\zeta = \zeta_1 + i\zeta_2$, where $\zeta_1$ and $\zeta_2$ are independent stochastic real variables with equal variances proportional to $\Gamma$.

From the Langevin equation we derive the associated FP equation that governs the time evolution of the probability density $\rho$. Using standard procedures [11], the resulting FP equation is

$$i\frac{\partial \rho}{\partial t} = \frac{\partial H}{\partial a}\frac{\partial \rho}{\partial a^*} - \frac{\partial H}{\partial a^*}\frac{\partial \rho}{\partial a} + i\frac{\partial}{\partial a}(\gamma g\rho + \frac{\Gamma}{2}\frac{\partial \rho}{\partial a^*}) + i\frac{\partial}{\partial a^*}(\gamma g^*\rho + \frac{\Gamma}{2}\frac{\partial \rho}{\partial a}). \tag{6}$$

Defining the Poisson brackets by

$$\{A, B\} = \frac{\partial A}{\partial a}\frac{\partial B}{\partial a^*} - \frac{\partial A}{\partial a^*}\frac{\partial B}{\partial a}, \tag{7}$$

the FP equation can be written as

$$i\frac{\partial \rho}{\partial t} = \{H, \rho\} - \{a, J^*\} - \{a^*, J\}, \tag{8}$$

where $J$ is the probability current, given by

$$J = i\gamma g\rho + i\frac{\Gamma}{2}\{a, \rho\}. \tag{9}$$

To determine $g$, we assume that the stationary solution of the FP equation is the Gibbs distribution given by

$$\rho_0 = \frac{1}{Z}e^{-\beta H}, \tag{10}$$

where $\beta = 1/kT$, and $T$ is the temperature. More precisely, we are supposing that the FP equation describes a system in contact with a heat reservoir at a temperature $T$. The Gibbs distribution is a stationary solution if $J(\rho_0) = 0$. Choosing $\Gamma = 2\gamma/\beta$, we find

$$g = \frac{\partial H}{\partial a^*}, \tag{11}$$

and the probability current (9) becomes

$$J = i\gamma g\rho + i\frac{\gamma}{\beta}\{a, \rho\}. \tag{12}$$

The last term of $J$ is the stochastic or noise term since it comes from the noise term of the Langevin equation

## 3 Quantum Fokker–Planck equation

The canonical form (8) of the FP equation is suitable for the canonical quantization, which is carried out by replacing a classical variable $A$ by an operator $\hat{A}$ acting on a Hilbert space and by replacing the Poisson brackets $\{A, B\}_{qp}$ by the commutator $[\hat{A}, \hat{B}]/i\hbar$, where $\hbar$ is the Planck constant. By this procedure, the relation $\{a, a^*\}_{q,p} = -i$ would give $[\hat{a}, \hat{a}^\dagger]$ equal to $\hbar$. However, as we wish this commutation to be equal to unity, that is, $[\hat{a}, \hat{a}^\dagger] = 1$, we use a rule in which $a$ is replaced with $\hat{a}\sqrt{\hbar}$ and $a^*$ with $\hat{a}^\dagger\sqrt{\hbar}$.

This rule is valid as long as we are using a representation in terms of real canonical variables such as the position $q$ and momentum $p$. If we are using a representation in terms of the complex canonical variable $a$ and $a^*$, then the appropriate procedure is to replace the Poisson brackets $\{A, B\}$ as defined by (7), with $[\hat{A}, \hat{B}]/\hbar$ because $\{A, B\} = i\{A, B\}_{q,p}$.

Using the procedure just explained, we are led to the following equation for the time evolution of the density operator $\rho$,

$$i\hbar\frac{\partial \rho}{\partial t} = [H, \rho] - [a, J^\dagger] - [a^\dagger, J], \tag{13}$$

where $H$ is the Hamiltonian, and $J$ is given by

$$J = i\gamma g\rho + \frac{i\gamma}{\beta}[a, \rho]. \tag{14}$$

We have also replaced $g$ with $g/\sqrt{\hbar}$ and have dropped the hats. The operator $a$ and its adjoint operator $a^\dagger$ are interpreted as the annihilation and creation operators, respectively, and $a^\dagger a$ is the number operator. As the last term in (12) is the noise term, the last term of (14) is the quantum noise term.

To find the operator $g$, we suppose that the stationary state is given the Gibbs density operator

$$\rho_0 = \frac{1}{Z} e^{-\beta(H - \mu a^\dagger a)}. \tag{15}$$

The Gibbs density operator (15) describes a system in contact with a heat reservoir at a temperature $T$ and in contact with a particle reservoir at a chemical potential $\mu$. The condition $J(\rho_0) = 0$ gives

$$g = \frac{1}{\beta}(e^{-\beta(H-\mu a^\dagger a)} a e^{\beta(H-\mu a^\dagger a)} - a). \tag{16}$$

The extension of the quantum FP Eq. (13) to the case of several interacting particles is given by

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] - \sum_j ([a_j, J_j^\dagger] + [a_j^\dagger, J_j]), \tag{17}$$

where

$$J_j = i\gamma_j \left( g_j \rho + \frac{1}{\beta_j}[a_j, \rho] \right), \tag{18}$$

and $\gamma_j$ and $\beta_j = 1/kT_j$ are parameters. The operator $g_j$ is defined by

$$g_j = \frac{1}{\beta_j}(e^{-\beta_j H_j} a_j e^{\beta_j H_j} - a_j), \tag{19}$$

where $H_j = H - \mu_j \hat{N}$, and

$$\hat{N} = \sum_j a_j^\dagger a_j \tag{20}$$

is the total number of particles operator. The operators $a_i$ and $a_i^\dagger$ represent the respective annihilation and creation of a particle in a one-particle state labeled by the index $i$. If we consider particles hopping on the sites of a lattice, the index $i$ denotes a site of the lattice, and $a_i$ and $a_i^\dagger$ annihilate and create a particle at the site $i$, respectively.

The quantum FP Eq. (17) is understood as describing a system in contact with several heat and particle reservoirs characterized by temperatures $T_j$ and chemical potentials $\mu_j$. The parameter $\gamma_j$ is understood as the strength of the contact of the system with the reservoir $j$.

If the temperatures are the same, $T_j = T$, and the chemical potentials are the same, $\mu_j = \mu$, then the stationary state is described by the Gibbs density operator

$$\rho_0 = \frac{1}{Z} e^{-\beta(H - \mu\hat{N})}. \tag{21}$$

This distribution leads to the vanishing of the term $[H, \rho_0]$ and of each current $J_j$, and thus represents not just a stationary state but a state of thermodynamic equilibrium. Indeed, in this case,

$$g_j = \frac{1}{\beta}(e^{-\beta(H-\mu\hat{N})} a_j e^{\beta(H-\mu\hat{N})} - a_j), \tag{22}$$

which can be written in the equivalent form

$$g_j \rho_0 + \frac{1}{\beta}[a_j, \rho_0] = 0, \tag{23}$$

from which we immediately see that $J_j(\rho_0) = 0$.

The quantum FP Eq. (17) is understood as appropriate for a collection of interacting particles. Up to this point we have not specified for which type of particles the equation is valid. We will show now that the equation is appropriate for bosons as well as fermions. Bosons obey the commutation relations $[a_k, a_\ell^\dagger] = \delta_{k\ell}$ and $[a_k, a_\ell] = 0$. To verify that these relations are indeed preserved by the quantum FP equation, we first determine the time evolution of the average

$$\langle F \rangle = \mathrm{Tr} F \rho \tag{24}$$

of any operator $F$. From the quantum FP Eq. (17), we find

$$i\hbar \frac{d}{dt}\langle F \rangle = \langle [F, H] \rangle + i \sum_j \gamma_j \langle g_j^\dagger [F, a_j] - [F, a_j^\dagger] g_j \rangle \\ - i \sum_j \frac{\gamma_j}{\beta_j} \langle [[F, a_j], a_j^\dagger] + [[F, a_j^\dagger], a_j] \rangle. \tag{25}$$

If we replace $F$ with $[a_k, a_\ell^\dagger]$, we see that both sides of Eq. (25) vanish. The same can be said if we replace $F$ with $[a_k, a_\ell]$.

Fermions obey the anti-commutation relations $a_k a_\ell^\dagger + a_\ell^\dagger a_k = \delta_{k\ell}$ and $a_k a_\ell + \sigma a_\ell a_k = 0$. To verify that the anti-commutation relations are preserved by the quantum FP equation, we replace $F$ with $a_k a_\ell^\dagger + a_\ell^\dagger a_k$. We see that both sides of Eq. (25) vanish. The same can be said if we replace $F$ with $a_k a_\ell + \sigma a_\ell a_k$. This shows that the quantum FP Eq. (17) is valid not only for bosons but also for fermions.

For convenience, we write down the commutation relation for bosons and the anti-commutation relation for fermions in the form

$$a_k a_\ell^\dagger - \sigma a_\ell^\dagger a_k = \delta_{k\ell}, \tag{26}$$

$$a_k a_\ell - \sigma a_\ell a_k = 0, \tag{27}$$

where $\sigma = 1$ for bosons and $\sigma = -1$ for fermions.

## 4 Quantum stochastic thermodynamics

Let us determine the time evolution of the energy $E = \langle H \rangle$ and of the average number of particles $N = \langle \hat{N} \rangle$. From the quantum FP equation we find

$$\frac{dE}{dt} = \Phi^e = \sum_j \phi_j^e, \tag{28}$$

where

$$\phi_j^e = -\frac{1}{i\hbar}\mathrm{Tr}([a_j, J_j^\dagger] + [a_j^\dagger, J_j])H, \tag{29}$$

which can be written as

$$\phi_j^e = \frac{1}{i\hbar}\mathrm{Tr}([a_j, H]J_j^\dagger + [a_j^\dagger, H]J_j). \tag{30}$$

In this form we see that it is understood as the flux of energy from the $j$ reservoir to the system.

The time evolution of the number of particles is

$$\frac{dN}{dt} = \Phi^n = \sum_j \phi_j^n, \tag{31}$$

where

$$\phi_j^n = -\frac{1}{i\hbar}\mathrm{Tr}([a_j, J_j^\dagger] + [a_j^\dagger, J_j])\hat{N}, \tag{32}$$

obtained by taking into account that $\hat{N}$ commutes with $H$. This expression can be written as

$$\phi_j^n = \frac{1}{i\hbar}\mathrm{Tr}([a_j, \hat{N}]J_j^\dagger + [a_j^\dagger, \hat{N}]J_j). \tag{33}$$

In this form we see that it is understood as the flux of particles from reservoir $j$ to the system.

The flux of heat from each reservoir is given by

$$\phi_j^q = \phi_j^e - \mu_j \phi_j^n, \tag{34}$$

where $\mu_j$ is the chemical potential related to reservoir $j$. The entropy flux from each reservoir is *assumed* to be given by

$$\phi_j = \frac{\phi_j^q}{T_j} = \frac{1}{T_j}\phi_j^e - \frac{\mu_j}{T_j}\phi_j^n, \tag{35}$$

where $T_j$ is the temperature of the reservoir $j$, and can be written as

$$\phi_j = -\frac{1}{i\hbar T_j}\mathrm{Tr}([a_j, J_j^\dagger] + [a_j^\dagger, J_j])(H - \mu_j \hat{N}). \tag{36}$$

The total entropy flux to the system is

$$\Phi = \sum_j \phi_j. \tag{37}$$

The time variation of the entropy of the system is not equal to the flux of entropy but includes a term due to entropy generation or entropy. Denoting by $\Pi$ the rate of entropy production, the time variation of the entropy $S$ of the system is

$$\frac{dS}{dt} = \Pi + \Phi. \tag{38}$$

In thermodynamic equilibrium, both $\Phi$ and $\Pi$ as well as $dS/dt$ vanish. In a nonequilibrium stationary state, $\Phi$ and $\Pi$ do not vanish, although $dS/dt$ does, in which case $\Pi = -\Phi$.

The entropy $S$ of the system is given by the von Neumann expression

$$S = -k\mathrm{Tr}\rho \ln \rho. \tag{39}$$

Deriving $S$ with respect to time and using the quantum FP equation, we find

$$\frac{dS}{dt} = \frac{k}{i\hbar}\sum_j \mathrm{Tr}([a_j, J_j^\dagger] + [a_j^\dagger, J_j]) \ln \rho. \tag{40}$$

An expression for $\Pi$ is obtained by subtraction $\Phi$, given by (36) and (37), from $dS/dt$, given by (40). The result is

$$\Pi = \frac{k}{i\hbar}\sum_j \mathrm{Tr}([a_j, J_j^\dagger] + [a_j^\dagger, J_j])(\ln \rho + \beta_j H - \beta_j \mu_j \hat{N}). \tag{41}$$

This expression can be written in the equivalent form

$$\Pi = \frac{k}{i\hbar}\sum_j \mathrm{Tr}([a_j, J_j^\dagger] + [a_j^\dagger, J_j])(\ln \rho - \ln \rho_j), \tag{42}$$

where

$$\rho_j = \frac{1}{Z_j}e^{-\beta_j (H - \mu_j \hat{N})}. \tag{43}$$

In the stationary state, the density $\rho$ will be independent of $t$ but it will not equal $\rho_j$, as these quantities are different, and we conclude that $\Pi$ will not vanish. However, if all the temperatures $T_j$ are the same and equal to $T$, and all chemical potentials $\mu_j$ are the same and equal to $\mu$, then $\rho_j$ are all equal to the Gibbs density

$$\rho_0 = \frac{1}{Z} e^{-\beta(H-\mu\hat{N})}, \tag{44}$$

and in this case the stationary density $\rho$ equals $\rho_0$ and $\Pi$ vanishes.

## 5 Noninteracting system

Let us consider a noninteracting system described by a Hamiltonian which is a sum of terms of the type $\varepsilon_j a_j^\dagger a_j$. As the particle do not interact, it suffices to treat just one of them. Thus we consider just one particle with Hamiltonian

$$H = \varepsilon a^\dagger a, \tag{45}$$

where we have dropped the index $j$. The system is in contact with a reservoir at temperature $T$ and chemical potential $\mu$. The quantum FP equation is given by Eqs. (13) and (14), and the operator $g$ by (16).

For $H = \varepsilon a^\dagger a$, the operator $g$ is proportional to $a$. To show this result, it suffices to determine $\langle n'|g|n\rangle$, where $|n\rangle$ are the eigenvectors of $a^\dagger a$, that is, $a^\dagger a|n\rangle = n|n\rangle$. Using the expression (16), we find

$$\langle n'|g|n\rangle = \frac{1}{\beta}(e^{-\beta(\varepsilon-\mu)(n'-n)} - 1)\langle n'|a|n\rangle. \tag{46}$$

Taking into account that $\langle n'|a|n\rangle$ is nonzero only when $n' = n - 1$, then

$$\langle n'|g|n\rangle = \frac{1}{\beta}(e^{\beta(\varepsilon-\mu)} - 1)\langle n'|a|n\rangle, \tag{47}$$

that is,

$$g = wa, \tag{48}$$

where

$$w = \frac{1}{\beta}(e^{\beta(\varepsilon-\mu)} - 1). \tag{49}$$

The time evolution of the average of any quantity $F$ is

$$i\hbar\frac{d}{dt}\langle F\rangle = \langle [F,H]\rangle + i\gamma(\langle g^\dagger [F,a]\rangle - \langle [F,a^\dagger]g\rangle) - \frac{i\gamma}{\beta}(\langle [[F,a],a^\dagger]\rangle + \langle [[F,a^\dagger],a]\rangle). \tag{50}$$

Replacing $F$ by $a^\dagger a$ in this equation, we find

$$\hbar\frac{d}{dt}\langle a^\dagger a\rangle = \frac{2\gamma}{\beta}\left(\sigma - e^{\beta(\varepsilon-\mu)}\right)\langle a^\dagger a\rangle + \frac{2\gamma}{\beta}, \tag{51}$$

where $\sigma = 1$ for bosons and $\sigma = -1$ for fermions.

In the stationary state, in fact, in equilibrium

$$\langle a^\dagger a\rangle = \frac{1}{e^{\beta(\varepsilon-\mu)} - \sigma}, \tag{52}$$

which is the mean occupation number. For bosons, $\sigma = 1$, the mean occupation number is

$$\langle a^\dagger a\rangle = \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}, \tag{53}$$

and for fermions, $\sigma = -1$, it is

$$\langle a^\dagger a\rangle = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}. \tag{54}$$

If we denote by $f = \langle a^\dagger a\rangle$ the mean occupation number, Eq. (51) becomes

$$\frac{d}{dt}f = -\alpha(f - f_0), \tag{55}$$

where $\alpha = 2\gamma/\beta\hbar f_0$, and $f_0$ is the mean occupation number at equilibrium, given by (52). The time-dependent solution is

$$f = f_0 + A_0 e^{-\alpha t}. \tag{56}$$

Next we determine the time-dependent solution of the quantum FP equation by assuming a solution of the type

$$\rho = \frac{1}{Z} e^{-Ba^\dagger a}, \tag{57}$$

where $B$ depends on $t$, and the normalization factor $Z$ is

$$Z = (1 - \sigma e^{-B})^{-\sigma}, \tag{58}$$

where $\sigma = 1$ for bosons and $\sigma = -1$ for fermions. The relation between $B$ and $f = \langle a^\dagger a\rangle$ is found by observing that

$$f = -\frac{\partial}{\partial B}\ln Z. \tag{59}$$

Therefore,

$$f = \frac{1}{e^B - \sigma}, \tag{60}$$

and the relation sought is

$$B = \ln(f^{-1} + \sigma). \tag{61}$$

As the time dependence of $f$ is known and given by (56), one concludes that $B$ is known as a function of $t$. Note that, when $t \to \infty$, $f \to f_0$ and $B \to \beta(\varepsilon - \mu)$, and we reach the equilibrium distribution

$$\rho_0 = \frac{1}{Z} e^{-\beta(\varepsilon-\mu)a^\dagger a}. \tag{62}$$

The entropy is determined by

$$S = -k\mathrm{Tr}\rho \ln \rho. \tag{63}$$

Using $\rho$ given by (57) and $B$ given by (61), we find $S$ as a function of $t$,

$$S = k(\sigma + f)\ln(1 + \sigma f) - kf \ln f. \tag{64}$$

The entropy flux $\Phi$ is obtained from the formulas (36) and (37), that is, by

$$\Phi = -\frac{1}{i\hbar T}(\varepsilon - \mu)\mathrm{Tr}(a^\dagger J - J^\dagger a), \tag{65}$$

and it is given by

$$\Phi = -k\alpha\beta(\varepsilon - \mu)(f - f_0), \tag{66}$$

valid for bosons and fermions.

To determine the rate of entropy production $\Pi$, we first determine $dS/dt$, which is given by (40), that is, by

$$\frac{dS}{dt} = \frac{k}{i\hbar}\mathrm{Tr}([a, J^\dagger] + [a^\dagger, J]) \ln \rho, \tag{67}$$

or by deriving (64) and using (55). The result is

$$\frac{dS}{dt} = -k\alpha(f - f_0) \ln \frac{1 + \sigma f}{f}. \tag{68}$$

Then we find the rate of entropy production by the difference $dS/dt - \Phi = \Pi$, which is

$$\Pi = k\alpha(f - f_0) \ln \frac{f + \sigma f f_0}{f_0 + \sigma f f_0}. \tag{69}$$

This expression is positive if $f > f_0$ or $f < f_0$, and vanishes when $f = f_0$, that is, in equilibrium, from which it follows that $\Pi \geq 0$. We recall that this expression is valid for bosons, $\sigma = 1$, and for fermions $\sigma = -1$.

## 6 Contact with two reservoirs

We consider here a simple system consisting of particles, either bosons or fermions, that hops between two sites labeled 1 and 2 and is in contact with two reservoirs. The site $j$ is in thermal contact with a heat reservoir $j$ at temperature $T_j$ and exchanges particles with the particle reservoir $j$ at the chemical potential $\mu_j$. The interacting Hamiltonian is

$$H = \varepsilon(a_1^\dagger a_1 + a_2^\dagger a_2) + \eta(a_1^\dagger a_2 + a_2^\dagger a_1), \tag{70}$$

and the FP equation is that given by Eq. (17) where $j$ takes only the values 1 and 2.

The total entropy flux is a sum of terms of the type (35) and is

$$\Phi = \frac{1}{T_1}\phi_1^e + \frac{1}{T_2}\phi_2^e - \frac{\mu_1}{T_1}\phi_1^n - \frac{\mu_2}{T_2}\phi_2^n, \tag{71}$$

where $\phi_j^e$ and $\phi_j^n$ are the fluxes of energy and particles from the reservoir $j$ to the system. We will consider only the stationary regime, in which case the fluxes are independent of time, and $\phi_1^e + \phi_2^e = 0$ and $\phi_1^n + \phi_2^n = 0$. In this case, $\Pi = -\Phi$, and we reach the following expression for the rate of entropy production

$$\Pi = \phi_e \chi_e + \phi_n \chi_n, \tag{72}$$

where $\phi_e = (\phi_1^e - \phi_2^e)/2$, $\phi_n = (\phi_1^n - \phi_2^n)/2$, and

$$\chi_e = \frac{1}{T_2} - \frac{1}{T_1}, \qquad \chi_n = \frac{\mu_1}{T_1} - \frac{\mu_2}{T_2}. \tag{73}$$

To determine the fluxes $\phi_j^e$ and $\phi_j^n$, we have to solve the quantum FP Eq. (17). To this end we need to determine $g_j$ given by Eq. (19). Using the same method employed in the previous section we find

$$g_1 = s_1 a_1 + r_1 a_2, \qquad g_2 = r_2 a_1 + s_2 a_2, \tag{74}$$

$$s_1 = \frac{1}{2}(w_1 + v_1), \qquad r_1 = \frac{1}{2}(w_1 - v_1), \tag{75}$$

$$r_2 = \frac{1}{2}(w_2 - v_2), \qquad s_2 = \frac{1}{2}(w_2 + v_2), \tag{76}$$

where

$$w_i = \frac{1}{\beta_i}(e^{\beta_i(\varepsilon_1 - \mu_i)} - 1), \tag{77}$$

$$v_i = \frac{1}{\beta_i}(e^{\beta_i(\varepsilon_2 - \mu_i)} - 1), \tag{78}$$

where $\varepsilon_1 = \varepsilon + \eta$ and $\varepsilon_2 = \varepsilon - \eta$.

The time evolution of the covariance $\langle a_1^\dagger a_1 \rangle = X_1$, $\langle a_2^\dagger a_2 \rangle = X_2$, $\langle a_1^\dagger a_2 \rangle = X_3 + iX_4$, and $\langle a_2^\dagger a_1 \rangle = X_3 - iX_4$ are obtained from Eq. (25). In the stationary state we find the equations

$$s_1 X_1 + r_1 X_3 - \frac{1}{c}X_4 = \frac{1}{\beta_1}(1 + (\sigma - 1)X_1), \tag{79}$$

$$s_2 X_2 + r_2 X_3 + \frac{1}{c}X_4 = \frac{1}{\beta_2}(1 + (\sigma - 1)X_2), \tag{80}$$

$$r_2X_1 + r_1X_2 + (s_1+s_2)X_3 = \left(\frac{1}{\beta_1}+\frac{1}{\beta_2}\right)(\sigma-1)X_3, \tag{81}$$

$$X_1 - X_2 - c(s_1+s_2)X_4 = \left(\frac{1}{\beta_1}+\frac{1}{\beta_2}\right)(\sigma-1)X_4, \tag{82}$$

where $c = \gamma/\eta$, and $\sigma = 1$ for bosons and $\sigma = -1$ for fermions.

Once the covariances are determined, the fluxes $\phi_j^e$ and $\phi_j^n$ are obtained from Eqs. (30) and (33), and we get

$$\phi_e = \frac{\gamma}{\hbar}[-(s_1\varepsilon - r_2\eta)X_1 - (r_1\eta - s_2\varepsilon)X_2 \\ - (s_1\eta + r_1\varepsilon)X_3 + (s_2\eta + r_2\varepsilon)X_3 + \frac{\varepsilon}{\beta_1} - \frac{\varepsilon}{\beta_2}], \tag{83}$$

$$\phi_n = \frac{\gamma}{\hbar}[-s_1X_1 + s_2X_2 - (r_1 - r_2)X_3 + \frac{1}{\beta_1} - \frac{1}{\beta_2}]. \tag{84}$$

Solving the equations for the covariances and replacing the solution in the above equations, we obtain the expression for the fluxes. From now on we obtain these expressions for the case where $\chi_e$ and $\chi_n$ are small. When they vanish, we find

$$X_1 = X_2 = \frac{1}{2}(f_1+f_2), \qquad X_3 = \frac{1}{2}(f_1 - f_2), \tag{85}$$

where

$$f_1 = \frac{1}{e^{\beta(\varepsilon_1-\mu)} - \sigma}, \qquad f_2 = \frac{1}{e^{\beta(\varepsilon_2-\mu)} - \sigma}, \tag{86}$$

and $X_4 = 0$, and $\phi_e = 0$ and $\phi_n = 0$. Here, $\beta$ and $\mu$ are defined by $\beta = (\beta_1+\beta_2)/2$ and $\mu = (\mu_1+\mu_2)/2$, and $\sigma = 1$ for bosons and $\sigma = -1$ for fermions.

The expansions of $\phi_e$ and $\phi_n$ up to linear terms in $\chi_e$ and $\chi_n$ are

$$\phi_e = K_{ee}\chi_e + K_{en}\chi_n, \tag{87}$$

$$\phi_n = K_{ne}\chi_e + K_{nn}\chi_n, \tag{88}$$

where the coefficients are

$$K_{ee} = \frac{\gamma T}{2\hbar}\{(1+f_1)\varepsilon_1^2 + (1+f_2)\varepsilon_2^2\}, \tag{89}$$

$$K_{en} = K_{ne} = \frac{\gamma T}{2\hbar}\{(1+f_1)\varepsilon_1 + (1+f_2)\varepsilon_2\}, \tag{90}$$

$$K_{nn} = \frac{\gamma T}{2\hbar}\{(1+f_1) + (1+f_2)\}. \tag{91}$$

These are known as the Onsager coefficients. We see that the diagonal coefficients are equal, in agreement with the Onsager reciprocal relations.

It is worth mentioning that when $T_1 = T_2$, the fluxes are proportional to $\mu_1 - \mu_2$,

$$\phi_e = C_e(\mu_1 - \mu_2), \tag{92}$$

$$\phi_n = C_n(\mu_1 - \mu_2), \tag{93}$$

where

$$C_e = \frac{\gamma}{2\hbar}\{(1+f_1)\varepsilon_1 + (1+f_2)\varepsilon_2\}, \tag{94}$$

$$C_n = \frac{\gamma}{2\hbar}\{(1+f_1) + (1+f_2)\}. \tag{95}$$

These quantities are finite even at zero temperature as long as $f_1$ and $f_2$ are finite. Thus, at zero temperature, there is a flux of particles as well as a flux of heat through the system if the chemical potentials are different.

## 7 Lindblad form

The quantum FP Eq. (17) is understood as a quantum Liouville equation supplemented by a term representing the dissipation and fluctuation, that is,

$$i\hbar\frac{\partial\rho}{\partial t} = [H,\rho] + i\mathcal{D}. \tag{96}$$

The dissipation-fluctuation term $\mathcal{D} = \mathcal{A} + \mathcal{B}$ is a sum of two parts,

$$\mathcal{A} = \alpha\sum_j([a_j, \rho h_j^\dagger] - [a_j^\dagger, h_j\rho]), \tag{97}$$

$$\mathcal{B} = \alpha\sum_j([a_j^\dagger, \rho a_j] - [a_j, a_j^\dagger\rho]), \tag{98}$$

where

$$h_j = e^{-\beta H}a_j e^{\beta H}, \tag{99}$$

and we are considering that the temperatures are all the same. These two terms can be written in the form

$$\mathcal{A} = \alpha\sum_j(a_j\rho h_j^\dagger + h_j\rho a_j^\dagger - \rho h_j^\dagger a_j - a_j^\dagger h_j\rho), \tag{100}$$

$$\mathcal{B} = \alpha\sum_j(2a_j^\dagger\rho a_j - \rho a_j a_j^\dagger - a_j a_j^\dagger\rho). \tag{101}$$

We wish to show that the dissipation-fluctuation have the Lindblad form [26]. The term $\mathcal{B}$ already has the Lindblad form, so our analysis is confined to the term $\mathcal{A}$. In the following we show that this term has the

Lindblad form when the Hamiltonian is bilinear in $a_j$ and $a_j^\dagger$,

$$H = \sum_{ij} H_{ij} a_i^\dagger a_j, \tag{102}$$

where $H_{ij}$ are $c$-numbers.

We start by considering a unitary transformation

$$a_j = \sum_k U_{jk} b_k, \qquad b_k = \sum_j U_{jk}^* a_j \tag{103}$$

where $U_{jk}$ are $c$-numbers with the property

$$\sum_k U_{ki}^* U_{kj} = \delta_{ij}, \tag{104}$$

and such that it diagonalizes $H$, transforming it into the form

$$H = \sum_k E_k b_k^\dagger b_k. \tag{105}$$

Using (103), we find

$$h_j = \sum_k U_{jk} q_k, \tag{106}$$

where

$$q_k = e^{-\beta H} b_k e^{\beta H}, \tag{107}$$

and $h_j$ transforms into $q_k$ like $a_j$ transforms into $b_j$. The terms $\mathcal{A}$ and $\mathcal{B}$ transform into

$$\mathcal{A} = \alpha \sum_k ([b_k, \rho q_k^\dagger] - [b_k^\dagger, q_k \rho]), \tag{108}$$

$$\mathcal{B} = \alpha \sum_k ([b_k, \rho b_k^\dagger] - [b_k^\dagger, b_k \rho]), \tag{109}$$

which have the same form as (97) and (98). Again, they can be written in a form similar to (100) and (101),

$$\mathcal{A} = \alpha \sum_k (b_k \rho q_k^\dagger + q_k \rho b_k^\dagger - \rho q_k^\dagger b_k - b_k^\dagger q_k \rho), \tag{110}$$

$$\mathcal{B} = \alpha \sum_j (2 b_k^\dagger \rho b_k - \rho b_k b_k^\dagger - b_k b_k^\dagger \rho). \tag{111}$$

The term $\mathcal{B}$ is again of the Linblad form as expected. To show that $\mathcal{A}$ is also of the Lindlad form, we use the property that $H$ has the diagonal form (105) in $b_k$. From this property, we find

$$q_k = e^{\beta E_k} b_k, \tag{112}$$

which when substituted in (110) gives

$$\mathcal{A} = \frac{\gamma}{\beta} \sum_k e^{\beta E_k} (2 b_k \rho b_k^\dagger - \rho b_k^\dagger b_k - b_k^\dagger b_k \rho), \tag{113}$$

which is of the Lindblad form.

For a Hamiltonian that is not bilinear in $a_j$ and $a_k^\dagger$, the method we use above is not appropriate. However, for a generic Hamiltonian, we may still use a canonical transformation. As the FP Eq. (96) is written in terms of commutators, its form will be preserved by a canonical transformation and so will the terms $\mathcal{A}$ and $\mathcal{B}$. If a canonical transformation exists that diagonalizes the Hamiltonian $H$, then the operator $q_k$, given by (107), reduces to the form (112), which makes the term $\mathcal{A}$ of the Lindblad form.

## 8 Conclusion

The canonical quantization procedure allowed us to obtain a quantum FP equation from the ordinary FP equation in terms of the creation and annihilation operators that is valid for bosons and fermions. The resulting equation is understood as a quantum Liouville equation supplemented by a dissipation term, as given by Eq. (96). The appropriate form of the dissipation term $D$ was established by imposing that in equilibrium, the density operator is of the Gibbs type.

When applied to noninteracting systems, we have obtained the time-dependent solution of the quantum FP equation from which we have obtained the mean occupation number and the rate of entropy production. In the stationary state, which means the equilibrium state, we have obtained the well-known expression for the mean occupation for bosons and for fermions.

Based on the quantum FP equations for several particles we have developed a quantum stochastic thermodynamics for nonequilibrium systems, and obtained the expressions for the rate of entropy production and the fluxes of heat and particles. The formalism was applied to a system in contact with two reservoirs from which we have obtained the fluxes of heat and particles, and the Onsager coefficients.

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