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Thermodynamics of Reduced State of the Field

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Abstract

Recent years have seen the flourishing of research devoted to quantum effects on mesoscopic and macroscopic scales. In this context, in *Entropy* 2019, *21*, 705, a formalism aiming at describing macroscopic quantum fields, dubbed Reduced State of the Field (RSF), was envisaged. While, in the original work, a proper notion of entropy for macroscopic fields, together with their dynamical equations, was derived, here, we expand thermodynamic analysis of the RSF, discussing the notion of heat, solving dynamical equations in various regimes of interest, and showing the thermodynamic implications of these solutions.

The Reduced State of the Field formalism

A set of bosonic modes in second quantization is described by the set of annihilation and creation operators $\hat{a}_k, \hat{a}_k^\dagger$ with commutation relations:

$$\left[\hat{a}_k, \hat{a}_{k'}^\dagger\right] = \delta_{kk'} \quad \left[\hat{a}_k, \hat{a}_{k'}\right] = \left[\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger\right] = 0$$

In the RSF formalism, the state $\hat{\rho}$ of the system is substituted by the couple $(\hat{r}, |\alpha\rangle)$:

$$\hat{r} = \sum_{k,k'} = \mathrm{Tr}\left[\hat{\rho}\hat{a}_{k'}^\dagger \hat{a}_k\right] |k\rangle\langle k'| \quad |\alpha\rangle = \sum_k \mathrm{Tr}[\hat{\rho}\hat{a}_k] |k\rangle$$

Operators in the original Fock space are put in correspondence with operators of the RSF according to:

$$\hat{B} = \sum_{k,k'} b_{kk'} \hat{a}_k^\dagger \hat{a}_{k'} \to \hat{b} = \sum_{k,k'} b_{kk'} |k\rangle\langle k'|$$
$$\hat{U} = e^{i\hat{B}} \to \hat{u} = e^{i\hat{b}}$$

Entropy in the RSF

The entropy of the RSF is defined as:

$$S[\hat{r}^\alpha] = \mathrm{tr}[(\hat{r}^\alpha + 1)\ln(\hat{r}^\alpha + 1) - \hat{r}^\alpha \ln \hat{r}^\alpha]$$

where the *correlation matrix* $\hat{r}^\alpha$ is defined as:

$$\hat{r}^\alpha = \hat{r} - |\alpha\rangle\langle\alpha| = \sum_{kk'} r_{kk'} - \alpha_k \alpha_{k'}^* |k\rangle\langle k'|$$

The entropy defined in this way is always greater or equal than zero, reaching its minimum value when the state of the RSF is coherent. Thus, the only pure states of the theory are the coherent states of the field.

Evolution of the RSF

The time evolution of the RSF assuming the most generic dynamics for the density matrix $\hat{\rho}$ can be written as:

$$\frac{d}{dt}\hat{r} = -\frac{i}{\hbar}[\hat{h}, \hat{r}] + (|\zeta\rangle\langle\alpha| + |\alpha\rangle\langle\zeta|) + \frac{1}{2}\{(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow), \hat{r}\} + \hat{\gamma}_\uparrow + \int \mu(du)(\hat{u}\hat{r}\hat{u}^\dagger - \hat{r})$$
$$\frac{d}{dt}|\alpha\rangle = -\frac{i}{\hbar}\hat{h}|\alpha\rangle + |\zeta\rangle + \frac{1}{2}(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow)|\alpha\rangle + \int \mu(du)(\hat{u} - 1)|\alpha\rangle$$

where the first term describes the free evolution, the second one the presence of a coherent field, the third term accounts for the presence of an environment and the last term can describe random scattering processes. The operator $\hat{\gamma}_\updownarrow$ is defined as:

$$\hat{\gamma}_\updownarrow = \sum_{k,k'} \Gamma_\updownarrow^{kk'} |k\rangle\langle k'|,$$

and it describes the absorption and emission of particles of the field from/into the environment according to the rates $\Gamma_\updownarrow^{kk'}$. As the entropy depends on the correlation matrix $\hat{r}^\alpha$, it is of interest to look at the evolution of this object:

$$\frac{d}{dt}\hat{r}^{(\alpha)} = -\frac{i}{\hbar}[\hat{h}, \hat{r}^{(\alpha)}] + \frac{1}{2}\left\{(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow), \hat{r}^{(\alpha)}\right\} + \hat{\gamma}_\uparrow$$
$$+ \int \mu(du)\left(\hat{u}\hat{r}^{(\alpha)}\hat{u}^\dagger - \hat{r}^{(\alpha)}\right) + \int \mu(du)(\hat{u} - 1)|\alpha\rangle\langle\alpha|(\hat{u}^\dagger - 1).$$

It is important to highlight that the dynamics of the correlation matrix does not depend on the presence of a coherent driving, which implies that the entropy is not influenced by the presence of a coherent driving.

Internal energy, work and heat

Once the entropy and its dynamics have been established, one should ask how the other important thermodynamic quantities should be defined in order to get a coherent description of thermodynamic phenomena. It turns that an appropriate definition of the internal energy is:

$$U = \mathrm{tr}\left[\hat{h}\hat{r}^\alpha\right]$$

In fact, using this definition one gets the expressions for work and heat:

$$d\,\mathrm{Tr}\left[\hat{h}\hat{r}^\alpha\right] = \mathrm{tr}\left[\frac{d\hat{h}}{dt}\hat{r}^\alpha\right] dt + \mathrm{tr}\left[\hat{h}\frac{\hat{r}^\alpha}{dt}\right] dt = dW + \delta Q$$

Quasi-static thermalization

For a quasi-static process, in which the state $\hat{\rho}$ is always in thermal equilibrium, the correlation matrix is always of the form

$$\hat{r}^{(\alpha)} = \frac{1}{e^{\beta\hat{h}} - 1}$$

Since in this case

$$\ln\left(\frac{\hat{r}^{(\alpha)} + 1}{\hat{r}^{(\alpha)}}\right) = \beta\hat{h},$$

we recover the equality from standard thermodynamics

$$dS = k_B \beta \delta Q.$$

This observation further strengthens our definition of work and heat. Moreover, for a non-quasi-static process, one has that $\hat{r}^{(\alpha)}$ is not of the form $\hat{r}^{(\alpha)} = (e^{\beta\hat{h}} - 1)^{-1}$, and thus one has also entropy production.

Thermalization under coherent driving

The correlation matrix of a system which is subject to a coherent driving and is also interacting with a thermal bath evolves according to:

$$\frac{\hat{r}^\alpha}{dt} = -\frac{i}{\hbar}[\hat{h}, \hat{r}^{(\alpha)}] + \frac{1}{2}\left\{(\hat{\gamma}_\uparrow - \hat{\gamma}_\downarrow), \hat{r}^{(\alpha)}\right\} + \hat{\gamma}_\uparrow$$

Assuming that the dynamics induced by the thermal bath is Markovian, it is easy to check that the steady state of the correlation matrix is given by:

$$r_{kk'}^{(\alpha)\mathrm{steady}} = \delta_{kk'} e^{-\beta\hbar\omega_k} Z_k = \frac{1}{e^{\beta\hat{h}} - 1}$$

From this result, one can see clearly that in presence of a thermal environment with temperature different from zero, it is impossible to obtain a coherent state, and that only an initial pure state remains pure. We can compute the steady state entropy as:

$$S[\hat{r}^{(\alpha)\mathrm{steady}}](\beta) = \beta U + \mathrm{tr}\left[\ln\left(\hat{r}^{(\alpha)\mathrm{steady}} + 1\right)\right]$$

from which we can define the equilibrium free energy as:

$$F_{\mathrm{eq}} = U[\hat{r}^{\alpha\mathrm{steady}}] - \beta^{-1} S[\hat{r}^{\alpha\mathrm{steady}}] = -\frac{1}{\beta}\mathrm{tr}\left[\ln\left(\hat{r}^{(\alpha)\mathrm{steady}} + 1\right)\right]$$

while for the non-equilibrium free energy we get:

$$F_{neq} = \mathrm{tr}\left[\hat{r}^{(\alpha)}\left(\hat{h} - \frac{1}{\beta}\ln\left(\frac{\hat{r}^{(\alpha)} + 1}{\hat{r}^\alpha}\right)\right)\right]$$

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