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Work distributions on Quantum Fields

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Abstract

In this thesis we tackle the problem of defining a notion of work distribution for non-equilibrium processes occurring in quantum fields. We study the work cost of processes in quantum fields without the need of projective measurements, which are always ill-defined in quantum field theory. Inspired by interferometry schemes, we propose a work distribution that generalizes the two-point measurement scheme employed in quantum thermodynamics to the case of quantum fields and avoids the use of projective measurements. The distribution is calculated for local unitary processes performed on KMS (thermal) states of scalar fields. Crooks theorem and the Jarzynski equality are shown to be satisfied, and some features of the resulting distributions are studied as functions of temperature and the degree of spatio-temporal localization of the unitary operation. We show how the work fluctuations become much larger than the average as the process becomes more localized in both time and space. This thesis led to one publication [1]

The thesis is structured as follows: In Chapter 1, a review of perturbation theory and some aspects of quantum field theory are included for completeness. In Chapters 2 and 3, we introduce the concepts of quantum thermodynamics and relativistic quantum information that we use in the derivations of our results. Chapter 4 is a summary of [1], which is included in the Appendix.

Keywords: Quantum fields, thermodynamics, causality, interferometry

Publications forming part of the thesis

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Contents

Chapter 1

Preliminaries

Throughout all this thesis, we work in units in which $c = \hbar = k_B = 1$

In this chapter we introduce the fundamental notions of perturbation theory and quantum field theory that are used throughout our work. There are many good books [2, 3] which explain in more detail and more thoroughly these concepts, that we review here for completeness.

1.1 Perturbation Theory

At the heart of Quantum Mechanics is the Schrodinger equation:

$$i\frac{d}{dt}\left|\psi(t)\right\rangle = \hat{H}(t)\left|\psi(t)\right\rangle \tag{1.1}$$

which describes the time evolution of quantum mechanical systems. It can easily be proven that the evolution generated by (1.1) is unitary:

$$\left|\psi(t)\right\rangle = \hat{U}(t,t_0)\left|\psi(t_0)\right\rangle, \tag{1.2}$$

where $\hat{U}(t,t_0)$ is a unitary operator satisfying $\hat{U}(t_0,t_0) = \mathbb{I}$ and $|\psi(t_0)\rangle$ is some initial condition. Using (1.1) a differential equation for the unitary operator $\hat{U}(t,t_0)$ can be obtained as well

$$i\frac{d}{dt}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0) \tag{1.3}$$

Despite being widely studied, the Schrodinger equation is yet far from being fully understood. Analytical solutions are only known for a handful of problems which describe very simple systems, involving few non-interacting particles and described by time-independent Hamiltonians $\hat{H}(t) = \hat{H}_0$. There are many problems of interest in which the Hamiltonian of the system can be written as a constant term plus a small perturbation, $\hat{H}(t) = \hat{H}_0 + \lambda\hat{V}(t)$, where λ is a small constant. In these cases, approximate solutions with different levels of accuracy can be obtained by expressing the unitary operator that dictates the time evolution as a power series in λ. We review here the theory behind this procedure, since in our work we will consider evolutions of quantum fields generated by perturbed Hamiltonians.

The Schrodinger and Heisenberg pictures

In an introductory Quantum Mechanics course, two ways of interpreting the time evolution of a quantum system are usually presented: the Schrodinger and the Heisenberg pictures. In the Schrodinger picture, the state vectors evolve with time while the operators are time independent:

$$\left|\psi(t)\right\rangle = \hat{U}(t,t_0)\left|\psi(t_0)\right\rangle. \tag{1.4}$$

The equation of motion obeyed by the state vectors is (1.1).

In the Heisenberg picture, the operators are the objects that change with time, with the state vectors remaining time independent. More precisely, if $\hat{U}(t,t_0)$ is the unitary evolution generated by the Hamiltonan $\hat{H}(t)$ between times t_0 and t, according to equation (1.1), and $\hat{O}(t)$ is a given operator, we would have that

$$\hat{O}_H(t) = \hat{U}^\dagger(t,t_0)\hat{O}(t)\hat{U}(t,t_0). \tag{1.5}$$

$\hat{O}_H(t)$ is the Heisenberg operator corresponding to the operator $\hat{O}(t)$, which corresponds to the operator in the Schrodinger picture. Note that we have included the possibility of $\hat{O}(t)$ being explicitly time dependent. We now obtain the equation of motion for $\hat{O}_H(t)$. Differentiating (1.5) and using (1.3) we obtain

$$\frac{d}{dt}\hat{O}_H(t) = i(\hat{U}^\dagger \hat{H}\hat{O}\hat{U} - \hat{U}^\dagger \hat{O}\hat{H}\hat{U}) + \hat{U}^\dagger \frac{\partial \hat{O}}{\partial t}\hat{U}. \tag{1.6}$$

Rewriting the right hand side in terms of the operators $\hat{O}$ and $\hat{H}$ written in the Heisenberg picture yields

$$\frac{d}{dt}\hat{O}_H(t) = i\Big[\hat{H}_H(t), \hat{O}_H(t)\Big] + \Big(\frac{\partial \hat{O}}{\partial t}\Big)_H. \tag{1.7}$$

The time derivative of the expectation value of an observable $\hat{O}$ has a similar structure in both the Schrodinger and Heisenberg pictures. We start by computing it in the Schrodinger picture:

$$\frac{d}{dt}\left\langle \hat{O} \right\rangle_t = \Big(\frac{\partial}{\partial t}\langle\psi(t)|\Big)\hat{O}\,|\psi(t)\rangle + \langle\psi(t)|\,\hat{O}\Big(\frac{\partial}{\partial t}|\psi(t)\rangle\Big) + \langle\psi(t)|\,\frac{\partial \hat{O}}{\partial t}\,|\psi(t)\rangle\,. \tag{1.8}$$

Using (1.1) gives

$$\frac{d}{dt}\left\langle \hat{O} \right\rangle_t = i\,\langle\psi(t)|\,(\hat{H}\hat{O} - \hat{O}\hat{H}\,|\psi(t)\rangle + \langle\psi(t)|\,\frac{\partial \hat{O}}{\partial t}\,|\psi(t)\rangle\,. \tag{1.9}$$

Therefore,

$$\frac{d}{dt}\left\langle \hat{O} \right\rangle_t = i\left\langle \Big[\hat{H}, \hat{O}\Big] \right\rangle_t + \left\langle \frac{\partial \hat{O}}{\partial t} \right\rangle_t. \tag{1.10}$$

To obtain the equivalent expression in the Heisenberg picture, the procedure is analogous. In this case we will use (1.3) instead of (1.1).

$$\frac{d}{dt}\left\langle \hat{O} \right\rangle_t = \langle\psi(t_0)|\,\frac{d\hat{O}_H}{dt}\,|\psi(t_0)\rangle = i\left\langle \Big[\hat{H}_H, \hat{O}_H\Big] \right\rangle_{t_0} + \left\langle \Big(\frac{\partial \hat{O}}{\partial t}\Big)_H \right\rangle_{t_0}. \tag{1.11}$$

The Dirac Picture

We are now going to introduce a framework that will be very useful to treat time-dependent problems. It is in between the Schrodinger and Heisenberg pictures, and it is known as the interaction or the Dirac picture. Both the states and the operators will depend on time, but on a carefully chosen way. Let the Hamiltonian of the system be

$$\hat{H}(t) = \hat{H}_0 + \lambda\hat{V}(t), \tag{1.12}$$

and let $\hat{U}_0 = e^{it\hat{H}_0}$ be the unitary transformation that transforms operators and states from the Schrodinger picture to the Dirac picture in the following way:

$$\hat{O}_D(t) = \hat{U}_0\hat{O}_S(t)\hat{U}_0^\dagger, \tag{1.13}$$

$$|\psi(t)\rangle_D = \hat{U}_0\,|\psi_s(t)\rangle\,, \tag{1.14}$$

where the subscripts D and S are used to denote operators and states in the Dirac and Schrodinger pictures, respectively. We will omit the subscript S from now on, as it should be clear from the context when we are referring to objects in the Schrodinger picture.

We now derive the expression for the Schrodinger equation in the Dirac picture. Starting from (1.1) and introducing the identity as $\hat{U}_0^\dagger\hat{U}_0$ we obtain,

$$i\frac{d}{dt}\big(\hat{U}_0^\dagger\hat{U}_0\,|\psi(t)\rangle\big) = \hat{U}_0^\dagger\hat{U}_0\hat{H}(t)\hat{U}_0^\dagger\hat{U}_0\,|\psi(t)\rangle\,.$$

Using the expressions for the operators and states in the Dirac picture, (1.13) and (1.14) gives

$$i\frac{d}{dt}\Big(\hat{U}_0^\dagger\,|\psi(t)\rangle_D\Big) = \hat{U}_0^\dagger\hat{H}_D(t)\,|\psi(t)\rangle_D\,.$$

From here, a few steps of calculations lead to the final expression

$$i\frac{d}{dt}\left|\psi(t)\right\rangle_D = \lambda V_D(t)\left|\psi(t)\right\rangle. \tag{1.15}$$

As we can see, the time evolution for the kets in the interaction picture is generated only by the time dependent part of the Hamiltonian.

Equation (1.15) has the same mathematical form as (1.1), so it should not be surprising that we can also write for a state $\left|\psi(t)\right\rangle_D$ in the interaction picture

$$\left|\psi(t)\right\rangle_D = \hat{U}_D(t,t_0)\left|\psi(t_0)\right\rangle_D, \tag{1.16}$$

where $\hat{U}_D(t,t_0)$ is a unitary operator. Substituting this into (1.15) we obtain a differential equation for the unitary operator $\hat{U}_D(t,t_0)$

$$\frac{d}{dt}\hat{U}_D(t,t_0) = -i\lambda\hat{V}_D(t)\hat{U}_D(t,t_0), \tag{1.17}$$

.

with the initial condition

$$\hat{U}_D(t,t_0) = \mathbb{I}. \tag{1.18}$$

Expressing (1.15) in integral form yields

$$\hat{U}_D(t,t_0) = \mathbb{I} - i\lambda\int_{t_0}^{t} \mathrm{d}t_1\hat{V}_D(t_1)\hat{U}_D(t_1,t_0). \tag{1.19}$$

By recursively substituting $\hat{U}_D(t,t_0)$ in the right hand side of the previous equation we obtain

$$\hat{U}_D(t,t_0) = \mathbb{I} - i\lambda\int_{t_0}^{t} \mathrm{d}t_1\hat{V}_D(t_1)\big(1 - i\lambda\int_{t_0}^{t_1} \mathrm{d}t_2\hat{V}_D(t_2)\big(1 - ... \tag{1.20}$$

When λ is much smaller than 1, from the previous expression we can derive the following power expansion for $\hat{U}_D(t,t_0)$

$$\hat{U}_D(t,t_0) = 1 + \hat{U}^{(1)}(t,t_0) + \hat{U}^{(2)}(t,t_0) + ... \tag{1.21}$$

where

$$\hat{U}_D^{(1)}(t,t_0) = -i\lambda\int_{t_0}^{t_1} \mathrm{d}t_1\hat{V}_D(t_1), \tag{1.22}$$

$$\hat{U}_D^{(2)}(t,t_0) = -\lambda^2\int_{t_0}^{t} \mathrm{d}t_1\int_{t_0}^{t_1} \mathrm{d}t_2\hat{V}_D(t_1)\hat{V}_D(t_2). \tag{1.23}$$

We will use these expression repeatedly in our work, as we will be mostly concerned with processes occurring in quantum fields arising from very small, local interactions. Usually (1.21) is written more succinctly as

$$\hat{U}_D(t,t_0) = \mathcal{T}\exp\left(-i\lambda\int_{t_0}^{t} \mathrm{d}t\hat{V}_D(t)\right), \tag{1.24}$$

where $\mathcal{T}$ refers to the time ordering operator.

1.2 Quantum Field Theory

We will now introduce the concepts of quantum field theory that are used in our work. We will first review some concepts of classical field theory and then we will show how to obtain a quantum field theory from a classical field theory by applying canonical quantization. We will mainly focus on the real scalar field, as this is the quantum field we study in our work.

Classical field theory

We can think of a classical field as a system described by a continuum of degrees of freedom $\phi(t, \mathbf{x})$, where in this case the position in space $\mathbf{x}$ is being used to index the different degrees of freedom. Our first goal will be to derive the equations of motion that will allow us to obtain the configuration of the field $\phi(t, \mathbf{x})$ at a time t, given its configuration at a time t_0, $\phi(t_0, \mathbf{x})$. The dynamics of a field are governed by a Lagrangian, which is a function of $\phi(t, \mathbf{x})$, $\dot{\phi}(t, \mathbf{x})$ and $\nabla\phi(t, \mathbf{x})$. In order to preserve locality, the Lagrangian at a time t will be the integral over space of a Lagrangian density, $L(t) = \int \mathrm{d}^3\mathbf{x}\mathcal{L}(\phi, \partial_\mu\phi)$. Furthermore, the Lagrangian density should be covariant, if we want our equations of motion to be consistent with special relativity. The equations of motion will be derived from the principle of least action, $\delta S = 0$ (where, $S = \int_{t_1}^{t_2} \mathrm{d}t L(t) = \int_{t_1}^{t_2} \mathrm{d}t \int \mathrm{d}^3\mathbf{x}\mathcal{L} = \int \mathrm{d}^4x\mathcal{L}$). For the particular case in which the Lagrangian density is that of the real scalar field,

$$\mathcal{L} = -\frac{1}{2}\partial^\mu\phi\partial_\mu\phi - \frac{1}{2}m^2\phi^2, \tag{1.25}$$

this would give

$$0 = \delta S = \int \mathrm{d}^4x\big[-\frac{1}{2}\partial^\mu\delta\phi\partial_\mu\phi - \frac{1}{2}\partial^\mu\phi\partial_\mu\delta\phi - \frac{1}{2}m^2\phi\delta\phi\big] = \int \mathrm{d}^4x\big[\partial^\mu\partial_\mu\phi - m^2\phi\big]\delta\phi, \tag{1.26}$$

where we have integrated by parts in each of the first two terms, and assumed that $\delta\phi$ vanishes at infinity on both the spatial and temporal dimensions, so that there is no surface term. The equation of motion resulting from (1.26) is therefore $-\partial^\mu\partial_\mu\phi + m^2\phi = 0$, which is known as the Klein-Gordon equation. Its general solution is

$$\phi(t, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}\sqrt{\omega_\mathbf{k}}}\big[a(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_\mathbf{k}t} - b(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x} + i\omega_\mathbf{k}t}\big], \tag{1.27}$$

where $a(\mathbf{k})$ and $b(\mathbf{k})$ are arbitrary functions, and $\omega_\mathbf{k} = (\mathbf{k}^2 + m^2)^{1/2}$. Particularizing to the case of a real field, we impose the additional condition $\phi(\mathbf{x}) = \phi^*(\mathbf{x})$. Using (1.27), the more general expression of a real scalar field reads

$$\phi(t, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}\sqrt{\omega_\mathbf{k}}}\big[a(\mathbf{k})e^{ikx} + a^*(\mathbf{k})e^{-ikx}\big], \tag{1.28}$$

where $kx = \mathbf{k}\cdot\mathbf{x} - \omega_\mathbf{k}t$. Now that we know the Lagrangian, we can also obtain the Hamiltonian following the usual procedure. Given a Lagrangian $L(q_i, \dot{q}_i)$, the conjugate momenta are given by $p_i = \frac{\partial L}{\partial \dot{q}_i}$, and the Hamiltonian by $H = \sum_i p_i\dot{q}_i - L$. As we discussed before, the generalized coordinates of a classical field are $\phi(t, \mathbf{x})$. That is, the role of q_i is played by $\phi(t, \mathbf{x})$. The appropriate generalizations are then

$$\Pi(\vec{x}) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}(\mathbf{x})}, \tag{1.29}$$

$$\mathcal{H} = \Pi\dot{\phi} - \mathcal{L}, \tag{1.30}$$

where $\mathcal{H}$ is the Hamiltonian density, and the Hamiltonian is the spatial integral of the Hamiltonian density. Obtaining the Hamiltonian for the real scalar field is very tedious and not very enlightening, so we will only include the expression for future reference.

$$H = \frac{1}{2}\int \mathrm{d}^3\mathbf{k}\omega_\mathbf{k}(a^*(\mathbf{k})a(\mathbf{k}) + a(\mathbf{k})a^*(\mathbf{k})). \tag{1.31}$$

Note that we do not add the terms inside the parenthesis. We do this in prevision of the following quantization of the real scalar field.

Quantum field theory

Now that we have a classical field theory, we can transform it into a quantum field theory by doing canonical quantization. This consists in upgrading the dynamical variables to operators and imposing commutation relations between them. There are several equivalent ways of doing so. In our case, we will set the commutation relations between $\hat{a}_\mathbf{p}$ and $\hat{a}^\dagger_\mathbf{q}$, and from here the rest of the relations can be obtained. The commutation relations between

the operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}^\dagger_{\mathbf{q}}$ (commonly referred to as annihilation and creation operators, respectively) are,

$$\begin{aligned}
&\left[\hat{a}_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{q}}\right] = 0, \\
&\left[\hat{a}^\dagger_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{q}}\right] = 0, \\
&\left[\hat{a}_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{q}}\right] = \delta^{(3)}(\mathbf{p}-\mathbf{q}).
\end{aligned} \tag{1.32}$$

As we said before, the operators $\hat{a}^\dagger_{\mathbf{q}}$ and $\hat{a}_{\mathbf{p}}$ are usually called creation and annihilation operators. This is because they behave in a very similar way as the creation and annihilation operators of the harmonic oscillator. Using them, we will be able to find a basis of eigenstates of the Hamiltonian, which as we remember from (1.31) is

$$\begin{aligned}
\hat{H} &= \frac{1}{2}\int \mathrm{d}^3\mathbf{k}\omega_{\mathbf{k}}(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \hat{a}_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}}) \\
&= \int \mathrm{d}^3\mathbf{k}\omega_{\mathbf{k}}(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \frac{1}{2}\delta^{(3)}(0)),
\end{aligned}$$

where we have used the commutation relation (1.32). The divergence at the origin is just a constant term that can be removed by changing the energy origin. The resulting Hamiltonian will then look like

$$\hat{H} = \int \mathrm{d}^3\mathbf{k}\omega_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}}. \tag{1.33}$$

We now proceed to find the eigenbasis of $\hat{H}$. We start by defining a vacuum state $|0\rangle$, with the property that it is annihilated by all the $\hat{a}_{\mathbf{k}}$, that is, $\hat{a}_{\mathbf{k}}|0\rangle = 0$ for all $\mathbf{k}$. This state has zero energy, as clearly $\hat{H}|0\rangle = 0$. The rest of the eigenstates of $\hat{H}$ are obtained by acting with the annihilation operators on the vacuum. From (1.32) and (1.33) it is easy to see that $\left[\hat{H}, \hat{a}^\dagger_{\mathbf{k}}\right] = \omega_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}}$. Therefore, $\hat{H}|\mathbf{k}\rangle = \omega_{\mathbf{k}}|\mathbf{k}\rangle$, and in general $\hat{H}|\mathbf{k}_1, ..., \mathbf{k}_n\rangle = (\omega_{\mathbf{k}_1} + ... + \omega_{\mathbf{k}_n})|\mathbf{k}_1, ..., \mathbf{k}_n\rangle$. The states of the form $|\mathbf{k}_1, ..., \mathbf{k}_n\rangle$ form an eigenbasis of the Hilbert space of the quantum field. From now on, when we talk about free scalar fields, we will be referring to the case in which the field is additionally massless ($m = 0$). This will help to simplify the notation.

Chapter 2

Quantum Thermodynamics

In our work, we extend two very important theorems of non-equilibrium statistical physics that had previously been proven for classical and finite dimensional quantum systems, to quantum fields. In this chapter, we introduce which are the theorems that we extend, and start to give some justifications of why the case of quantum fields is substantially harder than that of finite-dimensional quantum systems. These theorems were first introduced in classical non-equilibrium statistical physics, so we will start by reviewing the classical theory, and then move to the quantum case.

2.1 Classical Non-equilibrium Statistical Physics

Definitions

The state of a classical system is determined by a point $x = (q, p)$ in phase space. Suppose that our system is governed by a Hamiltonian of the form $H(x, \lambda)$, where λ is an externally controlled force parameter. This parameter λ will in general change with time, according to some previously specified protocol $\lambda(t)$. We will denote the trajectory followed by our system as $x_t = (q(t), p(t))$.

For a given trajectory x_t, we define the fluctuating work done on the system, and the fluctuated heat absorbed by the system, [4, 5] during the time interval $[0, \tau]$ as

$$W_{\tau,x_t} := \int_0^\tau \mathrm{d}t \frac{\partial H(x_t, \lambda(t))}{\partial \lambda(t)} \dot{\lambda}(t), \tag{2.1}$$

$$Q_{\tau,x_t} := \int_0^\tau \mathrm{d}t \frac{\partial H(x_t, \lambda(t))}{\partial x_t} \dot{x}_t. \tag{2.2}$$

They depend on the trajectory on the system in phase space, and correspond to the energy change due to the externally controlled force (work), and due to the response of the system's state (heat). Together they give the total change in the energy of the system, namely

$$W_{\tau,x_t} + Q_{\tau,x_t} = H(x_\tau, \lambda(\tau)) - H(x_0, \lambda(0)). \tag{2.3}$$

From now on, we will focus only in cases in which the system is closed. In these cases, all the change in energy is due to the work done on the system, since

$$Q_{\tau,x_t} = \int_0^\tau \mathrm{d}t \frac{\partial H(x_t, \lambda(t))}{\partial q(t)} \dot{q}(t) + \frac{\partial H(x_t, \lambda(t))}{\partial p(t)} \dot{p}(t) = \int_0^\tau -\dot{p}(t)\dot{q}(t) + \dot{q}(t)\dot{p}(t)\mathrm{d}t = 0. \tag{2.4}$$

So,

$$W = H(x_\tau, \lambda(\tau)) - H(x_0, \lambda(0)). \tag{2.5}$$

When we do not have perfect knowledge of the trajectory that our system follows, maybe because there is some uncertainty in the initial conditions, the work done on the system will not take a definite value, but it will become a random variable of the path followed in phase space x_τ. In this case, we have a probability density function over the paths $P(x_t)$ that the system follows. When the system is closed, every trajectory of the system is completely

determined by its initial conditions, so having a probability distribution over the space of all possible trajectories $P(x_t)$, is equivalent to having a probability density function over the set of initial conditions $P(x_0)$. Using (2.5), we can write the work probability distribution as

$$P(W) = \int P(x_0)\delta(W - (H(x_\tau, \lambda(\tau)) - H(z_0, \lambda(0))))\mathrm{d}x_0. \tag{2.6}$$

Now, the average value of the work done on the system is equal to the average final internal energy, minus the initial average internal energy:

$$\begin{aligned}\langle W_\tau^{closed}\rangle &= \int P(x_0)(H(x_\tau(x_0), \lambda(\tau)) - H(x_0, \lambda(0))\mathrm{d}x_0 \\ &= \int P_0(x_\tau)(H(x_\tau, \lambda(\tau))\Big|\frac{dx_0}{dx_\tau}\Big|\mathrm{d}x_\tau - \int P(x_0)H(x_0, \lambda(0))\mathrm{d}x_0 \\ &= U_\tau - U_0. \end{aligned}\tag{2.7}$$

The initial average internal energy is $U_0 = \int P(x_0)H(x_0, \lambda(0))\mathrm{d}x_0$, and the final average internal energy is $U_\tau = \int P_0(x_\tau)(H(x_\tau, \lambda(\tau))\mathrm{d}x_\tau = \int P_0(x_\tau)(H(x_\tau, \lambda(\tau))\Big|\frac{dx_0}{dx_\tau}\Big|\mathrm{d}x_\tau$ since Liouville's theorem implies that the determinant of the jacobian $\Big|\frac{dx_0}{dx_\tau}\Big| = 1$. In an experiment we would prepare the system in an initial configuration x_0 with probability $P(x_0)$, apply the force protocol $\lambda(t)$ to make the system evolve according to $H(x_t, \lambda(t))$ and measure the work done on the system for such execution of the protocol. By doing this repeatedly we can reconstruct the work probability distribution $P(W)$ of the process. We will use this idea greatly in the next section, when we will relate the work probability distribution $P(W)$ of certain processes with free energy differences ΔF of certain Gibbs states. The connection will be provided by two of the classical fluctuation theorems.

Classical fluctuation relations

We now present the two fluctuation theorems that we generalize to non-equilibrium processes occurring in quantum fields: the Jarzynski equality [6] and Crooks theorem [7]. They have been extensively used in non-equilibrium statistical physics to experimentally obtain differences of free energy between thermal states (see [8, 9, 10], for applications in biochemistry), that are otherwise hard to calculate or measure. They also have analogues for finite-dimensional quantum systems, that we will present in a later section.

We will start by stating and proving Jarzynski equality [6]. As before, we consider a closed system with Hamiltonian $H = H(x, \lambda)$, where λ is an externally tunable parameter that we change according to some prescribed protocol $\lambda(t)$, making the Hamiltonian time-dependent. For example, $H(x, \lambda) = \frac{p^2}{2m} + \frac{m\lambda^2 q^2}{2}$. In this case, λ is the frequency of the potential, that we can adjust. If the initial state of the system is the thermal state at some inverse temperature β of the initial Hamiltonian $H(x, \lambda(0))$, then, for any force protocol $\lambda(t)$, we have that

$$\langle e^{-\beta W_\tau^{closed}}\rangle = e^{-\beta\Delta F} \tag{2.8}$$

This result is known as Jarzynski equality. The left hand side is the expected value of $e^{-\beta W}$ when the initial state of the system is the thermal state at inverse temperature β of $H(x, \lambda(0))$, and a certain force protocol $\lambda(t)$ is applied on it. In the right hand side, the free energy difference is $\Delta F = F^\tau - F^0$, between the thermal states described by the Hamiltonian at the end of the force protocol, $H(x, \lambda(\tau))$, and at the beginning $H(x, \lambda(0))$. Note that if we apply two different force protocols $\lambda_1(t)$, $\lambda_2(t)$ such that $H(x, \lambda_1(0)) = H(x, \lambda_2(0))$ and $H(x, \lambda_1(\tau)) = H(x, \lambda_2(\tau))$, then in both cases $\langle e^{-\beta W_\tau^{closed}}\rangle$ are the same, since the initial and final thermal states defined by both protocols coincide. This can be used to experimentally obtain the free energy difference between to thermal states, by connecting them through a force protocol $\lambda(t)$ and use the method described in the previous section to reconstruct the work probability distribution (in this case, the probability distribution $P(x_0)$ would be $P(x_0) = \frac{e^{-\beta H(x_0, \lambda(0))}}{Z^{(0)}}$, where $Z^{(0)} = \int e^{-\beta H(x_0, \lambda(0))}\mathrm{d}x_0$ is the partition function of the corresponding thermal state). Jarzynski equality provides a deep connection between work probability distributions $P(W)$ arising in non-equilibrium processes, and free energy

differences of equilibrium states. It is a connection between non-equilibrium and equilibrium statistical physics. We now proceed to prove Jarzynski equality.

$$\langle e^{-\beta W_\tau^{closed}} \rangle = \int P(x_0) e^{-\beta W} \mathrm{d}x_0 = \int \frac{e^{-\beta H(x_0,\lambda(0))}}{Z^{(0)}} e^{-\beta(H(x_\tau,\lambda(\tau))-H(x_0,\lambda(0)))} \mathrm{d}x_0$$
$$\frac{1}{Z^{(0)}} \int e^{-\beta H(x_\tau,\lambda(\tau))} \left| \frac{dx_\tau}{dx_0} \right| \mathrm{d}x_\tau = \frac{Z^{(\tau)}}{Z^{(0)}} = e^{-\beta \Delta F}. \tag{2.9}$$

Another beautiful consequence of Jarzynski equality is that it implies the second law of thermodynamics. Applying Jensen's inequality to $\langle e^{-\beta W} \rangle$ gives $\langle e^{-\beta W} \rangle \geq e^{-\beta \langle W \rangle}$, so

$$\langle W \rangle \geq \Delta F \tag{2.10}$$

We now turn our attention to the second fluctuation theorem that we will extend to quantum field theory: Crooks theorem [7]. The setting is the same as for Jarzynski. Namely, we will study properties of work probability distributions arising in processes in which an initial thermal state is driven away from equilibrium by the action of some force protocol $\lambda(t)$. Crook's theorem states that

$$P^F(W) = P^B(-W) e^{\beta(W-\Delta F)}. \tag{2.11}$$

Here, $P^F(W)$ refers to the work probability distribution of a process in which the initial state is the Gibbs state of the Hamiltonian $H(x, \lambda(0))$ at inverse temperature β, and the force parameter λ is changed in the direction $\lambda(0) \to \lambda(\tau)$. This is the same process we considered when stating Jarzynski. We will refer to it as the forward process. $P^B(W)$ is the work distribution of a process that starts in a thermal state of the Hamiltonian $H(x, \lambda(\tau))$ at inverse temperature β, and the force parameter is changed in the direction $\lambda(\tau) \to \lambda(0)$. We will refer to it as the backward process. The proof of Crook's theorem is a bit more involved, and we will not include it here. We will just mention that Jarzynski equality (2.8) can be derived from Crooks theorem:

$$P^F(W) = P^B(-W) e^{\beta(W-\Delta F)} \Rightarrow P^F(W) e^{-\beta W} = P^B(W) e^{\beta \Delta D)}$$
$$\langle e^{-\beta W} \rangle = \int P^F(W) e^{-\beta W} \mathrm{d}W = e^{-\beta \Delta F}. \tag{2.12}$$

With this we finish our review of classical non-equilibrium statistical physics. In the next section, we move into the realm of quantum thermodynamics. Our goal will be to extend the validity of Jarzynski and Crooks theorems to quantum systems. However, this will not be easy. One difficulty is that for quantum systems the notion of of work becomes fuzzy. Unlike many other measurable quantities (position, momentum, energy...), work cannot be associated an observable [11]. This will make that we have to think more carefully the definition of work, even before we can start talking about fluctuation theorems. We will start treating these issues with more detail in the next section.

2.2 Quantum non-equilibrium statistical physics

Defining quantum fluctuating work

Every time we want to talk about some measurable quantity in quantum mechanics, we associate an observable to it. Some examples of this are energy, position, momentum, angular momentum... all these physical quantities have observables associated to them. One consequence of this is that the measurement process is local in time. The result of the measurement at time t only depends on the state of the system at that time, and not on how it arrived to such state. Indeed, energy, position, momentum... are magnitudes that also in classical physics can be determined only from the knowledge of the state of the system at the time that they are measured. However, as we learn in thermodynamics, the work done on a system depends in general on the trajectory that it follows. Even in the case of closed systems, the work will depend on the state of the system at two different instants of time.

We can start seeing that expressing work as an observable $\hat{W}$, such that $P(W) = \mathrm{Tr}\Big(\hat{W}\hat{\rho}\Big)$ will be problematic. This intuition can be made more rigorous [11].

One way of defining work in quantum systems is by looking more closely at expression (2.6). One can think of the work probability distribution (2.6) as being obtained by the following procedure:

1. Measure the energy of the initial state of the system $H(x_0, \lambda(0))$.
2. Let the system evolve according to the Hamiltonian $H(x_t, \lambda(t))$, starting from the initial condition x_0.
3. Measure the final energy of the system $H(x_\tau, \lambda(\tau))$.

The possible values of the work are $H(x_\tau, \lambda(\tau)) - H(x_0, \lambda(0))$, and the probability with which they are obtained is clearly given by (2.6). The advantage of thinking of (2.6) in this way is that it naturally yields an operational way of defining work distributions for quantum systems. What we will present now is known as the Two Point Measurement (TPM) scheme:

1. A projective measurement of $\hat{H}(0)$ is done on the initial state $\hat{\rho}$. This yields the energy measured as E_i and the post-measurement state $|E_i\rangle\langle E_i|$.
2. Unitary evolution of the post-measurement state according to the unitary associated to the process $\hat{U}(\tau, 0)$.
3. Finally, a projective measurement of $\hat{H}(\tau)$ is done on $\hat{U}(\tau,0)\,|E_i\rangle\langle E_i|\,\hat{U}^\dagger(\tau,0)$, returning the value E'_j.

The possible values of the work $w^{(ij)}$ are defined as $w^{(ij)} = E'_j - E_i$. The work probability distribution is

$$P(W) = \sum_{(ij)} \delta\left(W - w^{(ij)}\right) \langle E_i|\,\rho\,|E_i\rangle\,|\langle E'_j|\,\hat{U}(\tau,0)\,|E_i\rangle\,|^2, \tag{2.13}$$

From now on, we will denote $p_i = \langle E_i|\,\rho\,|E_i\rangle$ and $p_{j|i} = |\langle E'_j|\,\hat{U}(\tau,0)\,|E_i\rangle\,|^2$. The work distribution obtained through this prescription is usually denoted as P_{TPM}. It is worth noting that, when $[\hat{\rho}, \hat{H}(0)] \neq 0$ and $[\hat{H}(0), \hat{U}^\dagger \hat{H}(T)\hat{U}] \neq 0$, the statistics of the measurement of $\hat{H}(T)$ depend on whether we have measured the energy at time 0 or not. Also, in this case the expected value of the work according to P_{TPM} will not coincide with the difference in the internal energy of the system.

$$\sum_W P_{TPM}(W)W \neq \mathrm{Tr}\left(\hat{U}\hat{\rho}\hat{U}^\dagger\hat{H}(\tau)\right) - \mathrm{Tr}\left(\hat{\rho}\hat{H}(0)\right) \tag{2.14}$$

Essentially what this means is that the projective measurements have an invasive effect when the state of the system presents coherences the energy basis. This makes this definition of work not fully satisfactory. However, as we will see in the next section, this definition gives particularly good results when the initial state is diagonal in the energy basis. For instance, Jarzynski and Crooks theorems are recovered [12, 13, 14]. This is why this definition is widely used, and why coinciding with it in the case of initially diagonal states is a desirable property for any other definition of work distribution that may be proposed.

Different ways of defining work distributions for quantum systems have been proposed during the years [15]. The ultimate goal was to find a definition $P(W)$ that satisfied three physically well motivated properties:

1. There exists a POVM $\{\Pi_w\}$, dependent on $\hat{H}(0)$ and $\hat{H}(T), U$ but not on $\hat{\rho}$, such that $P(W) = \mathrm{Tr}(\hat{\rho}\Pi_w)$. Remember that a POVM $\{\Pi_w\}$ is a set of positive semidefinite operators Π_w that add up to the identity.
2. For all the states $\hat{\rho}$ such that $\Big[\hat{\rho}, \hat{H}(0)\Big] = 0$, $P(W) = P_{TPM}(W)$.
3. $\sum_W P(W)W = \mathrm{Tr}\left(\hat{U}\hat{\rho}\hat{U}^\dagger\hat{H}(\tau)\right) - \mathrm{Tr}\left(\hat{\rho}\hat{H}(0)\right)$.

However, it was recently proven [16] that it is impossible to find a definition of work distribution that simultaneously satisfies the three above mentioned properties. The idea of the proof is that Condition 2 essentially fixes the POVM elements to be those of the TPM scheme [17]. Condition 3 puts additional constraints on the POVM elements, and there can be found examples for which these constraints are not satisfied for the POVMs of the TPM scheme.

As we said, we will use the TPM scheme as our way to define work distributions , as it recovers the classical fluctuation theorems, and as we argued in the previous section, these can be used to experimentally determine many thermodynamic quantities of interest. We will now proceed to proof Jarzynski and Crooks theorem in the quantum regime.

Quantum Jarzynski and Crooks

We will start by proving the Jarzynski equality (2.8):

$$\langle e^{-\beta W}\rangle = \int P_{TPM}(W)e^{-\beta W}\mathrm{d}W = \sum_{i,j} p_i p_{j|i} e^{-\beta(E'_j - E_i)}. \tag{2.15}$$

When the initial state of the system $\hat{\rho}$ is a thermal state for the Hamiltonian $\hat{H}(0)$ at inverse temperature β:

$$\langle e^{-\beta W}\rangle = \sum_{i,j} \frac{e^{-\beta E_i}}{Z(0)} p_{j|i} e^{-\beta(E'_j - E_i)} = \frac{1}{Z(0)}\sum_{i,j} p_{j|i} e^{-\beta E'_j} = \frac{1}{Z(0)}\sum_j e^{-\beta E'_j} = \frac{Z(\tau)}{Z(0)} = e^{-\beta\Delta F}. \tag{2.16}$$

Here, we have used that $\sum_i p_{j|i} = \sum_i |\langle E'_j|\,\hat{U}(\tau,0)\,|E_i\rangle\,|^2 = 1$, since $\hat{U}(\tau,0)$ is unitary. The partition functions can be related to the free energies using the expression $F = -\frac{1}{\beta}\ln Z$.

Let us now proof Crooks theorem (2.11):

$$\begin{aligned} e^{-\beta W} P^F_{TPM}(W) &= \sum_{i,j} \delta(W - (E'_j - E_i)) e^{-\beta E'_j + \beta E_i} \frac{e^{-\beta E_i}}{Z(0)} |\langle E'_j|\,\hat{U}(\tau,0)\,|E_i\rangle\,|^2 \\ &= \frac{Z(\tau)}{Z(0)}\sum_{i,j} \delta(W - (E'_j - E_i)) \frac{e^{-\beta E'_j}}{Z(\tau)} |\langle E'_j|\,\hat{U}(\tau,0)\,|E_i\rangle\,|^2 \\ &= \frac{Z(\tau)}{Z(0)}\sum_{i,j} \delta(E_i - E'_j - W) \frac{e^{-\beta E'_j}}{Z(\tau)} |\langle E_i|\,\hat{U}^{-1}(\tau,0)\,|E'_j\rangle\,|^2 \end{aligned} \tag{2.17}$$

Remembering that

$$P^B_{TPM}(W) = \sum_{i,j} \delta(W - (E'_i - E'_j)) \frac{e^{-\beta E'_i}}{Z(\tau)} |\langle E'_i|\,\hat{U}^{-1}(\tau,0)\,|E_j\rangle\,|^2, \tag{2.18}$$

we can rewrite (2.17) as

$$e^{-\beta W} P^F_{TPM}(W) = \frac{Z(\tau)}{Z(0)} P^B_{TPM}(-W) = e^{-\beta\Delta F} P^B_{TPM}(-W), \tag{2.19}$$

concluding the proof of Crooks theorem for quantum systems.

Experimentally determining the work distribution $P_{TPM}(W)$ has not been possible until relatively recently [18], the reason being that doing projective measurements of quantum systems of high dimension is experimentally very difficult. The current methods to determine the work distribution use interferometric schemes, in which the system of interest is made to interact with a qubit in a prescribed way. The state of the qubit ends up encoding information about the work distribution, and in order to recover it we only have to do tomography of the state of the qubit. The first quantum fluctuation experiment was done in a nuclear magnetic resonance system.

Although these interferometric schemes were first introduced as a way to experimentally obtain work distributions, they will be a key ingredient of the definition of work distributions for quantum fields that we propose in [1] (a direct application of the TPM scheme is not possible, for reasons that we will explain in the next chapter). Therefore, we will explain

them now in a bit more of detail. Before we start, let us define first the characteristic function $\widetilde{P}(\mu)$ of a probability distribution $P(W)$ as

$$\widetilde{P}(\mu) = \int P(W) e^{i\mu W} \mathrm{d}W = \langle e^{i\mu W} \rangle \tag{2.20}$$

In the original proposals [19, 20], Ramsey interferometry was employed to probe the TPM work distributions as follows: the system of interest is coupled to an auxiliary qubit, which engages the system in an evolution conditional on whether the qubit is excited or not. By preparing the qubit in a superposition of ground and excited states, this process transfers the data about the characteristic function of the TPM work distribution to the state of the qubit. This is thus a rather 'non-invasive' procedure to acquire statistics which otherwise would require projective measurements. We summarize here the steps of the Ramsey scheme:

1. The system and the auxiliary qubit are prepared in the product state $\hat{\rho} \otimes |0\rangle\langle 0|$, where $\hat{\rho}$ is the state of the quantum system at the beginning of the thermodynamic process.
2. A Hadamard gate $\hat{H}$ is applied on the qubit.
3. The system and the auxiliary qubit evolve unitarily according to

$$\hat{M}_\mu = \hat{U}_S e^{-\mu \hat{H}_s(t_1)} \otimes |0\rangle\langle 0| + e^{-\mu \hat{H}_s(t_2)} \hat{U}_S \otimes |1\rangle\langle 1| \,. \tag{2.21}$$

   Here $\hat{U}_S$ is the unitary acting on the system between times t_1 and t_2.
4. A second Hadamard is applied to the qubit.

At the end of this procedure, we obtain that the reduced state of the auxiliary qubit is $\hat{\rho}_\mu = \frac{1}{2}\left(+ \mathrm{Re}(\widetilde{P}(\mu))\hat{\sigma}_z + \mathrm{Im}(\widetilde{P}(\mu))\hat{\sigma}_y \right)$. By iterating this process over many values of μ and performing state tomography, the work distribution of any unitary process on a system of interest may be non-projectively constructed. This has been experimentally implemented in [18].

When extending Jarzynsky ans Crooks theorem to non-equilibrium processes occurring on quantum fields, we stumble with two big difficulties. The first one, which we will now address, is that Jarzynski and Crooks theorem are statements about work probability distributions $P(W)$ generated when the initial sate of the system $\hat{\rho}$ is a Gibbs state, $\rho = \frac{e^{-\beta \hat{H}(0)}}{Z(0)}$. However, Gibbs states are not well defined in general when dealing with infinite-volume quantum systems (in particular quantum fields), as in those cases the partition function Z may not exist. We will have to use the notion of thermality captured by the Kubo-Martin-Schwinger (KMS) conditions. In the next section we will introduce these conditions and prove that the set of states that satisfy them (called KMS states) are an appropriate generalization of Gibbs states.

2.3 KMS states

We give here an introduction to KMS states [21, 22], that will be sufficient for our purposes. A more advanced treatment can be found in [23, 24]

Both in classical and quantum thermodynamics, thermal states are usually characterized using the notion of thermality given by Gibbs: thermal states are stationary states that maximize the entropy at constant energy. More formally, a state described by a density matrix $\hat{\rho}$ is thermal if it maximizes $S = -\mathrm{Tr}\left(\hat{\rho}\log(\hat{\rho})\right)$, subject to the constraints $\mathrm{Tr}\left(\hat{\rho}\right) = 1$ and $\mathrm{Tr}\left(\hat{\rho}\hat{H}\right) = E$. This gives rise to the familiar states of the form $\hat{\rho}_\beta = \frac{e^{-\beta \hat{H}}}{Z(\beta)}$.

However, when talking about infinite-volume quantum systems (in particular quantum fields) this notion of thermality turns out to be inadequate, as the partition function may not be defined. In this case, it is customary to use the notion of thermality captured by the Kubo, Martin and Schwinger (KMS) conditions. According to this conditions, $\hat{\rho}$ is a KMS state of inverse temperature β with respect to the time parameter τ parameterizing translations generated by a Hamiltonian $\hat{H}$ if and only if it satisfies the following two conditions for any pair of bounded Heisenberg picture operators $\hat{A}(\tau) = \hat{U}A(0)\hat{U}^\dagger$ and $\hat{B}(\tau) = \hat{U}B(0)\hat{U}^\dagger$ (where $\hat{U} = e^{i\hat{H}\tau}$).

1. The expectation values $\langle \hat{A}(0)\hat{B}(\tau)\rangle_\rho$ and $\langle \hat{B}(\tau)\hat{A}(0)\rangle_\rho$ are boundary values of some complex functions $\langle \hat{A}(0)\hat{B}(z)\rangle_\rho$ and $\langle \hat{B}(z)\hat{A}(0)\rangle_\rho$ holomorphic in the complex plane strips $0 < \mathrm{Im}\, z < \beta$ and $-\beta < \mathrm{Im}\, z < 0$, respectively.

2. The following complex anti-periodicity (of period β) is satisfied by the boundary values of these complex functions:

$$\langle \hat{A}(0)\hat{B}(\tau + i\beta)\rangle_\rho = \langle \hat{B}(\tau)\hat{A}(0)\rangle_\rho \tag{2.22}$$

The inclusion of the time parameter τ in the definition is not superfluous. KMS is an observer-dependent property, as well as the KMS inverse temperature β.

We will now prove some results that should help to solidify the idea that KMS states are the appropriate generalization of Gibbs states. We will start by seeing that all KMS states are stationary. Applying (2.22) to the particular choice of operators $\hat{A} = \mathbb{I}$ and $\hat{B}$ self-adjoint, we obtain that

$$\langle \hat{B}(\tau + i\beta)\rangle = \langle \hat{B}(0)\rangle, \tag{2.23}$$

which implies that $\langle \hat{B}(z)\rangle$ is periodic in the imaginary direction, with period $i\beta$. Applying Schwarz's inequality yields

$$|\langle \hat{B}(z)\rangle| \leq ||\hat{B}(z)|| = ||\hat{B}(x+iy)|| = ||e^{i\hat{H}x}\hat{B}(iy)e^{-i\hat{H}x}|| = ||\hat{B}(iy)||. \tag{2.24}$$

$\langle \hat{B}(z)\rangle$ is holomorphic, and (2.24) shows that it is bounded in the strip $0 < \mathrm{Im}z < \beta$. Due to its complex periodicity, $\langle \hat{B}(z)\rangle$ is also bounded in the rest of the complex plane. Applying Liouville's theorem (bounded entire functions are constant), we obtain that $\langle \hat{B}(z)\rangle$ is constant in the complex plane. In particular, $\langle \hat{B}(0)\rangle = \langle \hat{B}(\tau)\rangle$. Since $\hat{B}$ is an arbitrary observable, this proves that a KMS state is indeed stationary.

We will now prove that, when a partition function Z can be defined, a state $\hat{\rho}$ is a Gibbs state if and only if it is a KMS state. This is perhaps the most clear indication that KMS states are the right generalization of Gibbs states.

Lets first focus on the direction Gibbs $\Rightarrow$ KMS. Let $\hat{\rho}$ be a Gibbs state of inverse temperature β. We will see that $\hat{\rho}$ satisfies the two KMS conditions.

1. Condition 1. The operator

$$\hat{A}(0)\hat{B}(\tau + i\sigma)\hat{\rho} = \hat{A}(0)e^{-\sigma\hat{H}}\hat{B}(\tau)e^{-(\beta-\sigma)\hat{H}}/Z(\beta), \tag{2.25}$$

is of trace class [25] for $0 \leq \sigma \leq \beta$ because the operators on the right hand side are trace-class or bounded, and the product of a trace-class operator and a bounded operator is trace-class. As a consequence, in the complex strip $0 < \mathrm{Im}\, z < \beta$,

$$\langle \hat{A}(0)\hat{B}(z)\rangle_\rho = \mathrm{Tr}\left[\hat{A}(0)\hat{B}(0)\hat{\rho}\right], \tag{2.26}$$

is a well-defined function of z. In fact, it is a holomorphic function, as we will by checking that it satisfies the Cauchy-Riemann equations. (2.26) can be written as $f(z) = \mathrm{Tr}\Big(\hat{A}(0)e^{iz\hat{H}}\hat{B}(0)e^{-iz\hat{H}}\hat{\rho}\Big)$. Writing z as $z = \tau + i\sigma$, yields $\partial_\tau f = -i\partial_\sigma f$. The same reasoning can be applied to $\langle \hat{B}(z)\hat{A}(0)\rangle$. This proves that Gibbs states satisfy condition 1.

2. Condition 2. First, note that due to stationarity, the Hamiltonian cannot be time-dependent, so

$$\hat{B}(\tau) = e^{i\hat{H}\tau}\hat{B}(0)e^{-i\hat{H}\tau}. \tag{2.27}$$

Allowing τ to take complex values we get that

$$\hat{B}(\tau + i\beta) = e^{i\hat{H}(\tau+i\beta)}\hat{B}(0)e^{-i\hat{H}(\tau+i\beta)} = e^{-\beta\hat{H}}\hat{B}(\tau)e^{\beta\hat{H}}. \tag{2.28}$$

Substituting this and $\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Z(\beta)}$ in (2.22), and using the cyclic property of the trace:

$$\begin{aligned}\langle \hat{A}(0)\hat{B}(\tau + i\beta)\rangle_{\hat{\rho}} &= \mathrm{Tr}\left[\hat{A}(0)e^{-\beta\hat{H}}\hat{B}(\tau)e^{\beta\hat{H}}e^{-\beta\hat{Z}}\right]/Z(\beta) \\ &= \mathrm{Tr}\left[\hat{B}(\tau)\hat{A}(0)e^{-\beta\hat{H}}\right]/Z(\beta) = \mathrm{Tr}\left[\hat{B}(\tau)\hat{A}(0)\hat{\rho}\right] \\ &= \langle \hat{B}(\tau)\hat{A}(0)\rangle_{\hat{\rho}}.\end{aligned} \tag{2.29}$$

This completes the proof of Gibbs $\Rightarrow$ KMS.

We will now prove the converse, that KMS $\Rightarrow$ Gibbs when Gibbs states are well-defined. Let $\hat{\rho}$ be a KMS state of period β. Applying condition 2 at $\tau = 0$ we obtain that $\mathrm{Tr}\Big(\hat{A}(0)e^{-\beta\hat{H}}\Big[\hat{B}(0), e^{\beta\hat{H}}\hat{\rho}\Big]\Big) = 0$, for any bounded operator $\hat{A}$. This implies that $\Big[\hat{B}(0), e^{\beta\hat{H}}\hat{\rho}\Big] = 0$ for any bounded operator $\hat{B}$. Therefore, $e^{\beta\hat{H}}\hat{\rho}$ must be proportional to the identity $\Rightarrow$ $\hat{\rho}$ is a Gibbs state.

The last theorem should reassure us that KMS states are the correct generalization of Gibbs states for infinite-volume quantum systems. We will end by stating three more properties of KMS states that will be useful when working with KMS states in quantum field theory. For a KMS state $\hat{\rho}_\beta$ (with inverse KMS temperature β) with respect to time translations generated by a Hamiltonian $\hat{H}$ the two-point correlator $\mathcal{W}_{\hat{\rho}}(\tau, \tau') \coloneqq \mathrm{Tr}\left[\hat{\rho}\hat{\phi}\left(t\left(\tau\right)\boldsymbol{x}\left(\tau\right)\right)\hat{\phi}\left(t\left(\tau'\right)\boldsymbol{x}\left(\tau'\right)\right)\right]$ satisfies the following conditions:

1. $\mathcal{W}_\rho(\tau, \tau') = \mathcal{W}_\rho(\Delta\tau)$ (Stationarity).
2. $\mathcal{W}_\rho(\Delta\tau + \beta) = \mathcal{W}_\rho(-\Delta\tau)$ ($\mathbb{C}-$antiperiodicity).
3. Holomorphicity of the two-point correlator $\mathcal{W}_{\hat{\rho}}(0, z)$ in the upper complex strip $0 < \mathrm{Im}\, z < \beta$.

If we want to prove Jarzynski and Crooks theorems for non-equilibrium processes occurring in quantum fields with full generality, we will have to do it for the case in which the initial state of the system is a KMS state, and not simply a Gibbs state. One last problem that we should solve is how to define a work distribution in quantum field theory. Given the success that the TPM scheme has had reproducing fluctuation theorems in finite-dimensional quantum systems, it seems natural to also use the TPM scheme to define work distributions in quantum field theory. However, there is a problem with this approach. As we will explain in more detail in the next chapter, projective measurements cannot be allowed in a relativistic quantum theory, so readily applying the TPM scheme to quantum fields is not possible. We will explain how this problem is avoided in relativistic quantum information, and we will draw inspiration from here to define a work distribution using the Ramsey scheme introduced in this chapter.

Chapter 3

Relativistic Quantum Information

The focus of this chapter will be to introduce a way of measuring quantum fields that has been extensively used in the last years to show a wide variety of phenomena, such as entanglement harvesting [26, 27], communication through scalar fields [28]... and that is consistent with relativity. We will give two examples of how this formalism is applied: we will show that there is a non-zero probability of a detector jumping from the ground to the excited state when it is in contact with the vacuum state of a quantum field. We will also show that a detector that is in contact for a sufficiently long time with a quantum field in a KMS state will end up being in a thermal state. This is another proof that KMS states are the correct generalization of Gibbs states.

3.1 Measuring quantum fields

The question of how to measure a quantum field, was shown to be much more subtle than expected by Sorkin in [29]. He showed that, if we are allowed to do even localized projective measurements in a quantum field, we also have the possibility of doing faster than light communication. The way this is proven is by choosing three regions of spacetime O_1, O_2, O_3, so that some points of O_1 are in the causal past of some points of O_2, and some points of O_2 are in the causal past of some points of O_3, but O_1 and O_3 are spacelike separated. For general observables A, B, C measured in the regions O_1, O_2, O_3, respectively, and for a general state of the field $\hat{\rho}$, it can be proven that, if B is measured, the result of C depends on whether A was measured, even though A and C are spacelike separated. Therefore, by arranging that B will be measured with certainty, someone at O_1 could use this dependency of C on A to transmit information superluminally to O_3.

This result raised the question of which type of measurements could be done in quantum fields. A definite answer to this question was recently given by [30] in the context of algebraic quantum field theory, which is far beyond the scope of this text. The main idea is that measurements on a quantum field are made by interacting with the field on a finite region of spacetime using a probe, and measuring the probe afterwards. This technique had been used frequently in Relativistic Quantum Information, and many interesting effects such as entanglement harvesting [26, 27], communication through scalar fields [28], were studied using this procedure. Usually (although not always [31]), the quantum field to be measured will be a scalar field. In this case, it is customary to use as a probe a two-level system, whose interaction Hamiltonian with the field is given by (in the Dirac picture)

$$\hat{H}_{UDW}(t) = \lambda\chi(t)\int \mathrm{d}^3\mathbf{x} F(\mathbf{x})\hat{\mu}(t)\hat{\phi}(t,\mathbf{x}). \tag{3.1}$$

$\hat{\mu}(t) = \sigma^+ e^{i\Omega t} + \sigma^- e^{-i\Omega t}$ is the monopole operator, and $F(\mathbf{x})$ and $\chi(t)$ are the smearing and switching functions respectively. $F(\mathbf{x})$ represents the geometric shape of the two level system (also referred to as detector), and $\chi(t)$ the intensity and the duration of the coupling. Ω is the energy gap of the two-level system and σ^+ is the analogue of the $\hat{\sigma}_x$ operator ($\hat{\sigma}^- = \hat{\sigma}^{+\dagger}$). This model of interaction is known as the Unruh-DeWitt model, and is inspired in the light-matter interaction.

The main message to be taken away from this section is that quantum fields are measured using detectors. This is something that we will have to keep in mind when defining a notion of work distribution for quantum field theory. Such definition should not be based in the results of projective measurements directly applied on the field, but on the results collected when measuring detectors that have interacted with it.

We will now move on to prove that an Unruh-DeWitt detector that starts in its ground state $|g\rangle$ can be found with non-zero probability to be in its excited state $|e\rangle$ after interacting with the vacuum state of a scalar field.

Example 1: Excitations of UDW detectors

The Hamiltonian of the field and detector system is

$$\hat{H} = \hat{H}_f + \hat{H}_{TLS} + \hat{H}_{UDW}, \tag{3.2}$$

where $\hat{H}_f$ is the Hamiltonian of the free scalar field (1.12), $\hat{H}_{TLS}$ is the Hamiltonian of the two level system, $\hat{H}_{TLS} = \frac{\Omega}{2}\hat{\sigma}_Z$ and $\hat{H}_{UDW}$ is the Unruh-DeWitt Hamiltonian (3.1) that mediates the interaction between the two level system and the field. We will assume that λ is small, so that we can use perturbation theory in our calculations. We want to obtain $P^{|0\rangle}_{|g\rangle\to|e\rangle}(\Omega)$, namely the probability of the two level system of going from the ground to the excited state when it is in contact with the vacuum state of the free scalar field, as a function of the energy gap Ω. Clearly,

$$P^{|0\rangle}_{|g\rangle\to|e\rangle}(\Omega) = \sum_{out} |\langle out, e|\, \hat{U}\, |g, 0\rangle|^2 = \sum_{out} \langle 0, g|\, \hat{U}^\dagger\, |e, out\rangle \langle out, e|\, \hat{U}\, |g, 0\rangle\,, \tag{3.3}$$

where $\hat{U} = \mathcal{T}\exp\Big(\int_{-\infty}^{+\infty} \hat{H}_{UDW}(t)dt\Big)$, and the sum is done over all the possible final states of the field. Expanding $\hat{U}$ in power series as presented in (1.21), we obtain that

$$\begin{aligned} P^{|0\rangle}_{|g\rangle\to|e\rangle}(\Omega) &= \sum_{out} \langle 0, g|\, \mathbb{I} + \hat{U}^{\dagger(1)} + O(\lambda^2)\, |e, out\rangle \langle out, e|\, \mathbb{I} + \hat{U}^{(1)} + O(\lambda^2)\, |g, 0\rangle \\ &= \sum_{out} \langle 0, g|\, \hat{U}^{\dagger(1)}\, |e, out\rangle \langle out, e|\, \hat{U}^{(1)}\, |g, 0\rangle + O(\lambda^3). \end{aligned} \tag{3.4}$$

Here, we have used that the excited and ground states of the detector are orthogonal. Substituting the expression for $\hat{U}^{(1)}$ (1.22), and for $\hat{H}_{UDW}(t)$ (3.1) (remembering that the field $\hat{\phi}(\mathbf{x})$ is a free scalar field (1.28)) yields

$$P^{|0\rangle}_{|g\rangle\to|e\rangle}(\Omega) = \lambda^2 \int_{-\infty}^{+\infty} \mathrm{d}t \int_{-\infty}^{+\infty} \mathrm{d}t' \chi(t)\chi(t') \langle g|\, \hat{\mu}(t)\, |e\rangle \langle e|\, \hat{\mu}(t')\, |g\rangle \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}' \langle 0|\, \hat{\phi}(t, \mathbf{x})\hat{\phi}(t', \mathbf{x}')\, |0\rangle\,. \tag{3.5}$$

We now use the expressions of $\langle g|\, \hat{\mu}(t)\, |e\rangle = e^{-i\Omega t}$ and the two-point correlator of the field

$$\langle 0|\, \hat{\phi}(t, \mathbf{x})\hat{\phi}(t', \mathbf{x}')\, |0\rangle = \int \frac{\mathrm{d}^3\mathbf{k}}{2(2\pi)^3\omega_{\mathbf{k}}} e^{-i(\omega_{\mathbf{k}}(t-t') - \mathbf{k}\cdot(\mathbf{x}-\mathbf{x}'))}, \tag{3.6}$$

to obtain for the excitation probability of the detector

$$P^{|0\rangle}_{|g\rangle\to|e\rangle}(\Omega) = \lambda^2 \int \frac{\mathrm{d}^3\mathbf{k}}{2(2\pi)^3\omega_{\mathbf{k}}} |\widetilde{\chi}(\Omega + \omega_{\mathbf{k}})|^2 |\widetilde{F}(\mathbf{k})|^2, \tag{3.7}$$

where $\widetilde{\chi}$ and $\widetilde{F}$ are the Fourier transforms of the switching and smearing functions. As we can see, there is a non-zero probability for the detector to jump to the excited state.

We will now pause for a moment to explain why this result is counter-intuitive. The Unruh-DeWitt model is a simplified model for the light matter interaction. However, for certain physical scenarios, such as those considered in quantum optics, this model can still be unnecessarily complex. In theses cases, usually, two further assumptions are performed: the single mode approximation and the rotating wave approximation [32]. When these approximations are made, the final Hamiltonian for the light-matter interaction is that of the Jaynes-Cummings model

$$\hat{H}_{JC} = \lambda(\hat{\sigma}^+\hat{a}_\Omega + \hat{\sigma}^-\hat{a}^\dagger_\Omega). \tag{3.8}$$

The interpretation of this Hamiltonian is clear. The two level system can go from the ground to the excited state by absorbing a photon whose energy equals its energy gap Ω (this is the term $\hat{\sigma}^{+}\hat{a}_{\Omega}$). Conversely, if the two level system starts in the excited state, it can deexcite emitting a photon in the process. As we can see, with this model of interaction, it is impossible that the two-level system goes from the ground to the excited state if it interacts with a field that is in its vacuum state (no photons), as opposed to what we see if we use the Unruh-DeWitt detector model. This is just an example of a series of features of the light-matter interaction that appear when we use the UDW model, but not under certain additional approximations [33].

We will now see another example of how to use detectors to establish properties of quantum fields.

Example 2: Thermalization of an UDW detector

We will show that, under certain conditions, an Unruh-DeWitt detector that interacts for a long time with a KMS state of a scalar field, will end up being in a thermal state. In order to prove this, we will show that

$$\frac{P_{exc}(\Omega)}{P_{deexc}(\Omega)} = e^{-\beta\Omega}, \tag{3.9}$$

where β is the inverse temperature of the KMS state of the field, and $P_{exc}(\Omega)$ and $P_{deexc}(\Omega)$ are the excitation and deexcitation probabilities of the detector when it is in contact with the field. For simplicity, we will assume that the detector is pointlike, that is $F(\mathbf{x}) = \delta^{(3)}(\mathbf{x})$. Also, we will introduce a timescale σ, that will control the duration of the interaction.

Particularizing (3.5) to the case of a point-like detector, we have that $P(\Omega) = \lambda^2\sigma\mathcal{F}(\Omega,\sigma)$, where

$$\mathcal{F}(\Omega,\sigma) = \frac{1}{\sigma}\int_{-\infty}^{+\infty}\mathrm{d}\tau\int_{-\infty}^{+\infty}\mathrm{d}\tau'\chi\Big(\frac{\tau}{\sigma}\Big)\chi\Big(\frac{\tau'}{\sigma}\Big)e^{i\Omega(\tau-\tau')}\mathcal{W}(\tau,\tau'), \tag{3.10}$$

$\mathcal{W}_{\hat{\rho}}(\tau,\tau') = \mathrm{Tr}\left[\hat{\rho}\hat{\phi}\left(t\left(\tau\right)\boldsymbol{x}\left(\tau\right)\right)\hat{\phi}\left(t\left(\tau'\right)\boldsymbol{x}\left(\tau'\right)\right)\right]$ and $\hat{\rho}$ is the state of the field. Now we write $\chi(\frac{\tau}{\sigma})$ as

$$\chi\Big(\frac{\tau}{\sigma}\Big) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega\widetilde{\chi}(\omega)e^{-i\omega\frac{\tau}{\sigma}}, \tag{3.11}$$

and

$$\chi\Big(\frac{\tau}{\sigma}\Big) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega\widetilde{\chi}^{*}(\omega)e^{i\omega\frac{\tau}{\sigma}}. \tag{3.12}$$

Therefore,

$$\mathcal{F}(\Omega,\sigma) = \frac{1}{4\pi^2\sigma}\int_{-\infty}^{+\infty}\mathrm{d}\tau\int_{-\infty}^{+\infty}\mathrm{d}\tau'\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\widetilde{\chi}^{*}(\omega)\widetilde{\chi}(\omega')e^{i(\frac{\omega\tau}{\sigma}-\frac{\omega'\tau'}{\sigma})}\mathcal{W}(\tau,\tau')e^{i(\tau-\tau')\Omega}. \tag{3.13}$$

Since the field is in a KMS state with respect to τ, it is also stationary with respect to τ, $\mathcal{W}(\tau,\tau') = \mathcal{W}(\tau-\tau')$. By doing the change of variables

$$\begin{aligned} u &= \tau - \tau' \\ v &= \tau + \tau' \end{aligned} \tag{3.14}$$

we can rewrite (3.13) as

$$\begin{aligned} \mathcal{F}(\Omega,\sigma) &= \frac{1}{8\pi^2\sigma}\int_{-\infty}^{+\infty}\mathrm{d}u\int_{-\infty}^{+\infty}\mathrm{d}v\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\widetilde{\chi}^{*}(\omega)\widetilde{\chi}(\omega')e^{i(\frac{\omega u}{2\sigma}+\frac{\omega' u}{2\sigma})}e^{i(\frac{\omega v}{2\sigma}-\frac{\omega' v}{2\sigma})}\mathcal{W}(u)e^{iu\Omega} \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}u\int_{-\infty}^{+\infty}\mathrm{d}\omega|\widetilde{\chi}(\omega)|^2\mathcal{W}(u)e^{i(\Omega+\frac{\omega}{\sigma})u} \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega|\widetilde{\chi}(\omega)|^2\widetilde{\mathcal{W}}\Big(\Omega+\frac{\omega}{\sigma}\Big). \end{aligned} \tag{3.15}$$

We want the limit of long interactions (large σ). If $\widetilde{\chi}(\omega)$ decays fast enough, we arrive to

$$\lim_{\sigma\to\infty}\mathcal{F}(\Omega,\sigma)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega|\widetilde{\chi}(\omega)|^2\widetilde{\mathcal{W}}(\Omega)=\frac{\widetilde{\mathcal{W}}(\Omega)}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega|\widetilde{\chi}(\omega)|^2=\widetilde{\mathcal{W}}(\Omega). \tag{3.16}$$

Now, using the $\mathbb{C}-$antiperiodicity of the two-point correlator of KMS states

$$\mathcal{W}(\Delta\tau+i\beta)=\mathcal{W}(-\Delta\tau)\Rightarrow\int_{-\infty}^{+\infty}\mathrm{d}\Delta\tau\mathcal{W}(\Delta\tau+i\beta)e^{i\omega\Delta\tau}=\int_{-\infty}^{+\infty}\mathrm{d}\Delta\tau\mathcal{W}(-\Delta\tau)e^{i\omega\Delta\tau}. \tag{3.17}$$

The RHS is equal to $\widetilde{\mathcal{W}}(-\omega)$. For the LHS, we do the change of variables $\Delta\tau'=\Delta\tau+i\beta$ and integrate ver the $\mathrm{Im}\,z=i\beta$ line:

$$\int_{-\infty}^{+\infty}\mathrm{d}\Delta\tau\mathcal{W}(\Delta\tau+i\beta)e^{i\omega\Delta\tau}=\int_{\gamma}\mathrm{d}\Delta\tau'\mathcal{W}(\Delta\tau')e^{i\omega(\Delta\tau'-i\beta)}=e^{\beta\omega}\int_{\gamma}\mathrm{d}\Delta\tau' e^{i\omega\Delta\tau'}=e^{\beta\omega}\widetilde{\mathcal{W}}(\omega). \tag{3.18}$$

For the last step we have used the holomorphicity of the two-point correlator $\mathcal{W}_{\hat{\rho}}(0,z)$ in the upper complex strip $0<\mathrm{Im}\,z<\beta$ and Cauchy integral theorem.

Putting everything together, we have that

$$\frac{P_{exc}(\Omega)}{P_{deexc}(\Omega)}=\frac{\mathcal{F}(\Omega,\sigma)}{\mathcal{F}(-\Omega,\sigma)}=\frac{\widetilde{\mathcal{W}}(\Omega)}{\widetilde{\mathcal{W}}(-\Omega)}=e^{-\beta\omega}, \tag{3.19}$$

as desired.

With this we conclude our section of examples on how to use detectors to study non-trivial properties of quantum fields. In the next chapter, we will use this idea to defnie a notion of work distribution for quantum fields, that will satisfy Crooks and Jarzynski theorems.

Chapter 4

Work distributions on quantum fields

In this chapter we will summarize the results obtained in [1]. The complete article is included in the Appendix.

Our objective is to extend Crooks and Jarzynski theorems to non-equilibrium processes occurring in quantum fields. There are two main difficulties for doing so. First, if we want our results to be general, we will have to work with KMS states, and not simply with Gibbs states. Second, we cannot readilty extend the TPM scheme to quantum field theory, as it involves doing projective measurements of a quantum field. We have to define a work distribution based on the results of measurements done in detectors.

In Chapter 2 we introduced the Ramsey scheme, as a way of experimentally obtaining the work distribution for processes occurring in finite-dimensional quantum systems. It involved a controlled interaction of a qubit and the system of interest, and later by measuring the state of the qubit the characteristic function of the work distribution could be obtained. This is precisely the type of operational schemes that we need to define a work distributions in quantum fields avoiding projective measurements, and is actually the way we define it. In [1] we operationally define work distributions of quantum fields through the Ramsey scheme, and then start studying its properties.

We study work distributions of processes whose Hamiltonians are of the form

$$\hat{H}_\phi(t) = \hat{H}_0 + \lambda\chi(t)\int_{\mathbb{R}^3} \mathrm{d}^3\boldsymbol{x} F(\boldsymbol{x})\hat{\phi}(t,\boldsymbol{x}) = \hat{H}_0 + \hat{H}_I(t), \tag{4.1}$$

in the interaction picture, where $\hat{H}_0$ is the free Hamiltonian of the field (1.33). We assume that the switching function has strong support in a finite region and, without loss of generality, we take the strong support of the switching function to be in the interval $[0,T]$, where 0 and T are the starting and ending times of the process under study. Assuming that the coupling constant λ is small, we can use perturbation theory to obtain closed expressions for the characteristic function of the work distribution to second order in λ, for an arbitrary KMS state of the massless free scalar field:

$$\begin{aligned}\widetilde{P}(\mu) = 1 + \lambda^2 \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}\left(e^{\beta\omega_{\boldsymbol{k}}}-1\right)} |\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2 |\widetilde{F}(\boldsymbol{k})|^2 \times \left(e^{\beta\omega_{\boldsymbol{k}}}+1\right)\left(\cos(\mu\omega_{\boldsymbol{k}})-1\right) \\ + i\lambda^2 \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}} |\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2 |\widetilde{F}(\boldsymbol{k})|^2 \sin(\mu\omega_{\boldsymbol{k}}).\end{aligned} \tag{4.2}$$

Now that we have a closed expression for the characteristic function, we will try to prove Jarzynski and Crooks theorems. Since we are considering cyclic processes ($\hat{H}(0) = \hat{H}(T)$), Jarzynski equality reads in this case $\langle e^{-\beta W}\rangle = 1$. By evaluating $\widetilde{P}(\mu)$ at $i\beta$ we obtain the desired result. Now, to prove Crooks theorem we have to do the inverse Fourier transform of (4.2) to recover the work probability distribution $P(W)$

$$P(W) = (1-p)\delta(W) + \frac{\lambda^2}{2\pi}|\widetilde{\chi}(W)|^2 |\widetilde{F}(W)|^2 W \times \left(\frac{e^{\beta W}}{e^{\beta W}-1}\Theta(W) + \frac{1}{1-e^{-\beta W}}\Theta(-W)\right), \tag{4.3}$$

where $p \coloneqq \int_{W\neq 0} \mathrm{d}W P(W)$ and $\Theta(W)$ is the Heaviside function. It is just a calculation to check that $\frac{P(W)}{P_{rev}(-W)} = e^{\beta W}$.

With this we have proved that for unitaries generated by Hamiltonians of the form (4.1), our definition of work distribution satisfies Jarzynski and Crooks theorems. This, together with the definition of $P(W)$ for quantum fields through the Ramsey scheme, are the two main results of [1]. We also study some features of the work probability distribution (4.3). Of significant interest is to understand when the work fluctuations dominate the work average values. From the characteristic function (4.2) it is possible to obtain by differentiation the different moments of $P(W)$. We find that, for the vacuum ($\beta = \infty$)

$$\langle W \rangle = \lambda^2 \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2} |\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2 |\widetilde{F}(\boldsymbol{k})|^2, \tag{4.4}$$

$$\sigma_\beta^2 = \frac{\lambda^2}{2} \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} \frac{e^{\beta\omega_{\boldsymbol{k}}}+1}{e^{\beta\omega_{\boldsymbol{k}}}-1} |\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2 |\widetilde{F}(\boldsymbol{k})|^2 \omega_{\boldsymbol{k}} + \mathcal{O}(\lambda^4). \tag{4.5}$$

An interesting observation is that, for the vacuum, if we consider unitaries that are very localized in time and space, both $\widetilde{\chi}(\omega_{\boldsymbol{k}})$ and $\widetilde{F}(\boldsymbol{k})$ will be wide in the frequency space, which means that the work variance will become larger than the expectation value, making the variance of the work increasingly significant as the operation on the field becomes increasingly localized in both time and space. Several other observations about the work distribution (4.3) can be made. We refer the reader to [1] for a deeper analysis.

Future work could involve use our definition of work distribution to study the thermodynamics of processes of interest occurring in quantum fields, such as entanglement harvesting, quantum energy teleportation [34]... Also, it could be interesting to relate the work done in the system with the variation of internal energy in adiabatic and non-adiabatic processes.

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Work distributions on quantum fields

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We study the work cost of processes in quantum fields without the need of projective measurements, which are always ill-defined in quantum field theory. Inspired by interferometry schemes, we propose a work distribution that generalizes the two-point measurement scheme employed in quantum thermodynamics to the case of quantum fields and avoids the use of projective measurements . The distribution is calculated for local unitary processes performed on KMS (thermal) states of scalar fields. Crooks theorem and the Jarzynski equality are shown to be satisfied, and some features of the resulting distributions are studied as functions of temperature and the degree of spatio-temporal localization of the unitary operation. We show how the work fluctuations become much larger than the average as the process becomes more localized in both time and space.

Introduction.- One of the key features of thermal and statistical physics at the microscopic scale is that average quantities no longer characterize completely the state of a system or the features of a thermodynamic process. In these regimes, stochastic or quantum fluctuations become relevant, being of the same order of magnitude as the expectation values [1–3]. It is therefore important to develop tools that allow us to study the properties of these fluctuations, so as to have a complete picture of thermodynamics at the small scales.

One of the best studied quantities in this context is work of out of equilibrium processes, and its associated fluctuations. The notion of work is a paramount empirical cornerstone of macroscopic equilibrium thermodynamics. However, work in microscopic quantum scenarios is a notoriously subtle concept (for instance, it cannot be associated to an observable [4]), and although there is not a single definition of work distributions and work fluctuations in quantum theory, several possibilities have been proposed (see [5] for a detailed comparison). Perhaps the most established notion of work fluctuations is that defined through the Two-Point Measurement (TPM) scheme [6], where the work distribution of a given process is obtained by performing two projective measurements of the system's energy, at the beginning and at the end of the process. The TPM formalism defines a work distribution that has a number of desirable properties: it is linear on the input states, it agrees with the unambiguous classical definition for states diagonal in the energy eigenbasis, and it yields a number of fluctuation theorems in different contexts [1, 7].

An important caveat of this definition is that it cannot be straightforwardly generalized to processes involving quantum fields: projective measurements in quantum field theory (QFT) are incompatible with its relativistic nature. They can introduce ill-defined operations due to UV divergences and, among other serious problems, enable superluminal signaling even in the most innocent scenarios [8]. For these reasons, it has been strongly argued that projective measurements should be banished from the formalism of any relativistic field theory, even in the case that the projective measurements are performed over spacetime localized observables [8–10]. However, quantum fields are certainly subject to a wealth of thermodynamic and non-equilibrium phenomena, and as such it should be possible to define an operationally meaningful work distribution, potentially different from the standard TPM scheme. One avenue to build such a work distribution is through the ability to operate on quantum fields through locally coupling other systems, such as e.g., atoms or particle detectors. This allows the performance of (non-projective) measurements on the field that are well-defined [11] and physically meaningful [12]. Thus, whichever definition we construct for the work distribution, it should be based on such physically attainable localized measurements, and should not rely on projective measurements as some previous works attempted (e.g., [13]).

In recent works [14, 15], it was shown that the complete work distribution given by TPM scheme for a finite dimensional system can be easily measured by performing measurements on an auxiliary qubit, in what is called a Ramsey interferometric scheme. This was first experimentally implemented in [16]. Inspired by this idea, we propose a definition of a work distribution in quantum fields based on the Ramsey scheme, which, as we will show, is in fact well defined for a QFT despite the impossibility of projective measurements. We show that this new distribution (that generalizes the TPM scheme in the absence of projective measurements) satisfies the usual Jarzynski and Crooks theorems when the field is initially in a KMS state (the states that generalize thermal Gibbs states for quantum fields [17, 18]) and evolves through a spatially localized unitary. This shows that such work distribution is well-defined for fields even though projective measurements are not. We also obtain analytical expressions for the variance and the average of the work distribution for some useful simple cases of local field operations. Finally we discuss how, through either Crooks or Jarzynski's theorems, the proposed work distribution

can be used as a new way of computing ratios of partition functions between field theories that can potentially yield simpler approaches to the problem than path integral methods.

TPM work distributions and Ramsey scheme.- We focus on processes defined by a state of a quantum system $\hat{\rho}$ initially in an equilibrium KMS state of temperature β^{-1}, which is driven out of equilibrium by a time-dependent Hamiltonian $\hat{H}(t)$, turned on during an interval $[0,T]$. The work distribution quantifies the work cost of the unitary process on the field $\hat{U}(T,0)$ generated by the Hamiltonian $\hat{H}(t)$.

As mentioned above, projective measurements, even when localized in a compact region of space and free of divergences, cannot be implemented in quantum fields because they are incompatible with relativistic causality [8–10]. Thus, the TPM scheme cannot be readily applied to processes involving quantum fields. However, as we show, the Ramsey scheme, which only involves interactions with a low-dimensional ancilla, provides an indirect way to gather the same work statistics. For completeness, let us review the TPM scheme to define a work distribution. The steps are the following:

1. A projective measurement of $\hat{H}(0)$ is done on the initial state $\hat{\rho}$. This yields the energy measured as E_i and the post-measurement state $|E_i\rangle\langle E_i|$.

2. Unitary evolution of the post-measurement state according to the unitary associated to the process $\hat{U}(T,0)$.

3. Finally, a projective measurement of $\hat{H}(T)$ is done on $\hat{U}(T,0)\,|E_i\rangle\langle E_i|\,\hat{U}^\dagger(T,0)$, returning the value E'_j.

The possible values of the work $w^{(ij)}$ are defined as $w^{(ij)} = E'_j - E_i$. The work probability distribution is

$$P(W) = \sum_{(ij)} \delta\left(W - w^{(ij)}\right) \langle E_i|\,\rho\,|E_i\rangle\,|\langle E'_j|\,\hat{U}(T,0)\,|E_i\rangle\,|^2, \tag{1}$$

with a corresponding characteristic function

$$\widetilde{P}(\mu) = \int P(W) e^{\mathrm{i}\mu W} dW = \langle e^{i\mu W}\rangle. \tag{2}$$

It is also important to define a "time-reversed" process, in which the driving has the opposite temporal order. That is,

1. A projective measurement is done on the basis of $\hat{H}(T)$, yielding $E'_{j,\mathrm{rev}}$.

2. The unitary evolution $\hat{U}_{\mathrm{rev}}(T,0)$ corresponding to the driven Hamiltonian $\hat{H}(T-t)$ with $t=[0,T]$ is implemented.

3. A final projective measurement in the basis of $\hat{H}(0)$ is implemented returning the value $E_{i,\mathrm{rev}}$.

The corresponding work probability distribution is

$$P_{\mathrm{rev}}(W) = \sum_{(ij)} \delta\left(W - w^{(ji)}_{\mathrm{rev}}\right) \times \langle E'_{j,\mathrm{rev}}|\,\rho\,|E'_{j,\mathrm{rev}}\rangle\,|\langle E_{i,\mathrm{rev}}|\,\hat{U}(T,0)\,|E'_{j,\mathrm{rev}}\rangle\,|^2, \tag{3}$$

where $w^{(ji)}_{\mathrm{rev}} = E_{i,\mathrm{rev}} - E'_{j,\mathrm{rev}}$. We can also define $\widetilde{P}_{\mathrm{rev}}(\mu) = \int P_{\mathrm{rev}}(W) e^{\mathrm{i}\mu W} dW$.

In the original proposals [14, 15], Ramsey interferometry was employed to probe the TPM work distributions as follows: the system of interest is coupled to an auxiliary qubit, which engages the system in an evolution conditional on whether the qubit is excited or not. By preparing the qubit in a superposition of ground and excited states, this process transfers the data about the characteristic function of the TPM work distribution to the state of the qubit. This is thus a rather 'non-invasive' procedure to acquire statistics which otherwise would require projective measurements. The steps are:

1. The system and the auxiliary qubit are prepared in the product state $\hat{\rho}\otimes|0\rangle\langle 0|$, where $\hat{\rho}$ is the state of the quantum system at the beginning of the thermodynamic process.

2. A Hadamard gate is applied on the qubit.

3. The system and the auxiliary qubit evolve unitarily according to

$$\hat{M}_\mu = \hat{U}_S e^{-\mathrm{i}\mu\hat{H}(0)} \otimes |0\rangle\langle 0| + e^{-\mathrm{i}\mu\hat{H}(T)}\hat{U}_S \otimes |1\rangle\langle 1|\,. \tag{4}$$

   Here $\hat{U}_S$ is the unitary acting on the system between times 0 and T.

4. A second Hadamard is applied to the qubit.

At the end of this procedure, we obtain that the reduced state of the auxiliary qubit is $\hat{\rho}_\mu = \frac{1}{2}\left(\mathbb{1} + \mathrm{Re}(\widetilde{P}(\mu))\hat{\sigma}_z + \mathrm{Im}(\widetilde{P}(\mu))\hat{\sigma}_y\right)$. By iterating this process over many values of μ and performing state tomography, the work distribution of any unitary process on a system of interest can then be constructed without projective measurements.

Work distributions for thermal states of quantum fields.- Since projective measurements on quantum fields are not allowed, we design a version of the Ramsey scheme to obtain a characteristic function that defines the work distribution of a process, which will be a localized unitary on a scalar field. Consider a scalar quantum field $\hat{\phi}(t,\boldsymbol{x})$ written in terms of plane-wave modes as

$$\hat{\phi}(t,\boldsymbol{x}) = \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^{3/2}\sqrt{2\omega_{\boldsymbol{k}}}} \left(\hat{a}_{\boldsymbol{k}} e^{\mathrm{i}\mathsf{k}\cdot\mathsf{x}} + \hat{a}^\dagger_{\boldsymbol{k}} e^{-\mathrm{i}\mathsf{k}\cdot\mathsf{x}}\right), \tag{5}$$

where $\mathsf{k}\cdot\mathsf{x} := \boldsymbol{k}\cdot\boldsymbol{x} - \omega_{\boldsymbol{k}}t$, $\omega_{\boldsymbol{k}} = \sqrt{m^2+\boldsymbol{k}^2}$ and $\left[\hat{a}_{\boldsymbol{p}}, \hat{a}^\dagger_{\boldsymbol{q}}\right] = \delta^{(3)}(\boldsymbol{p}-\boldsymbol{q})$. We take the field to be in a KMS state [17, 18] of inverse temperature β, $\hat{\rho}_\beta$. KMS thermality generalizes Gibbs' notion of thermality to cases where, due to the dimensionality of the Hilbert space, Gibbs thermal states are not well-defined. This is the case of QFTs, where usually the partition function is ill-defined. More formally, for a KMS state $\hat{\rho}_\beta$ (with inverse KMS temperature β) with respect to time translations generated by a Hamiltonian $\hat{H}$ the two-point correlator $\mathcal{W}_{\hat{\rho}}(\tau,\tau') := \mathrm{Tr}\left[\hat{\rho}\hat{\phi}\left(t\left(\tau\right)\boldsymbol{x}\left(\tau\right)\right)\hat{\phi}\left(t\left(\tau'\right)\boldsymbol{x}\left(\tau'\right)\right)\right]$ satisfies the following two conditions (see, among many others, [19, 20]):

1. $\mathcal{W}_\rho(\tau,\tau') = \mathcal{W}_\rho(\Delta\tau)$ (Stationarity).

2. $\mathcal{W}_\rho(\Delta\tau + \mathrm{i}\beta) = \mathcal{W}_\rho(-\Delta\tau)$ ($\mathbb{C}-$antiperiodicity).

Notice that the vacuum state is a KMS state with $\beta\to\infty$, that is, zero temperature.

We proceed to characterize the localized unitary we apply on the field. For a free scalar field, any local observable is a linear combination of the field amplitude $\hat{\phi}$ and its canonical momentum $\hat{\pi}$. For concreteness, in this letter, we focus on unitaries acting on the field that are generated by Hamiltonians of the form

$$\hat{H}_\phi(t) = \hat{H}_0 + \lambda\chi(t)\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{x}F(\boldsymbol{x})\hat{\phi}(t,\boldsymbol{x}) = \hat{H}_0 + \hat{H}_I(t), \tag{6}$$

in the interaction picture, where $\hat{H}_0$ is the free Hamiltonian of the field, and $\chi(t)$ and $F(\boldsymbol{x})$ are the switching and smearing functions, respectively. We assume that the switching function has strong support in a finite region [21] and, without loss of generality, we take the strong support of the switching function to be in the interval $[0,T]$, where 0 and T are the starting and ending times of the process under study. In other words, the field evolves freely (or very approximately freely if the switching function is not strictly compact) except for the interval $[0,T]$ where we perform a spatiotemporally localized unitary operation on the support of $F(\boldsymbol{x})$. By doing this, we obtain that $\hat{H}_\phi(0) = \hat{H}_\phi(T) = \hat{H}_0$, which simplifies our analysis. This is a particular unitary operation on a localized field observable (that represents, in the language of quantum optics, a multimode displacement operation [22]). Considering localized unitaries generated by a smeared $\hat{\pi}$ is completely analogous, so this particular case is easily generalizable to all localized unitaries on a free field.

At the beginning of the Ramsey scheme, the state of the field-qubit system is $\hat{\rho} = \hat{\rho}_\beta\otimes|0\rangle\langle 0|$. Applying the Hadamard on the qubit results in $\hat{\rho}_0 = \hat{\rho}_\beta\otimes|+\rangle\langle+|$. We apply the controlled unitary evolution

$$\hat{M}_\mu = \hat{U}_\phi(T)e^{-\mathrm{i}\mu\hat{H}_0}\otimes|0\rangle\langle 0| + e^{-\mathrm{i}\mu\hat{H}_0}\hat{U}_\phi(T)\otimes|1\rangle\langle 1|\,, \tag{7}$$

where $\hat{U}_\phi(T)$ is the unitary on the field generated by the Hamiltonian (6), given by

$$\hat{U}_\phi(T) = \mathcal{T}\exp\left(-\mathrm{i}\lambda\int_{\mathbb{R}}\mathrm{d}t\,\chi(t)\int_{\mathbb{R}^3}\mathrm{d}^3\boldsymbol{x}\,F(\boldsymbol{x})\hat{\phi}(t,\boldsymbol{x})\right), \tag{8}$$

where $\mathcal{T}$ represents time-ordering. Assuming that the coupling λ is small enough, we can obtain an approximate expression for $\hat{U}_\phi(T)$ through a Dyson expansion: $\hat{U}_\phi(T) = \mathbb{1} + \hat{U}^{(1)} + \hat{U}^{(2)} + \mathcal{O}(\lambda^3)$, where in the interaction picture

$$\hat{U}^{(1)} = -\mathrm{i}\lambda\int_{\mathbb{R}}\mathrm{d}t\,\hat{H}_I(t),\ \hat{U}^{(2)} = -\lambda^2\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{t}\mathrm{d}t'\hat{H}_I(t)\hat{H}_I(t'). \tag{9}$$

The reduced state of the qubit at time T can be written as $\hat{\rho}_T = \hat{\rho}_T^{(0)} + \hat{\rho}_T^{(1)} + \hat{\rho}_T^{(2)} + \mathcal{O}(\lambda^3)$, where $\hat{\rho}_T^{(i)}$ is proportional to λ^i. The explicit expression can be found in the Appendix.

$\mathrm{Tr}[\hat{\sigma}_z\hat{\rho}_\mu]$ and $\mathrm{Tr}[\hat{\sigma}_y\hat{\rho}_\mu]$ give the real and imaginary parts, respectively, of the characteristic function (2). Using the KMS two-point correlator (see e.g., [23]), we can write the characteristic function for this process as

$$\begin{aligned}\widetilde{P}(\mu) := 1 + \lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}\left(e^{\beta\omega_{\boldsymbol{k}}}-1\right)}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2 \\ \times\left(e^{\beta\omega_{\boldsymbol{k}}}+1\right)\left(\cos(\mu\omega_{\boldsymbol{k}})-1\right) \\ + \mathrm{i}\lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2\sin(\mu\omega_{\boldsymbol{k}}).\end{aligned} \tag{10}$$

By taking the inverse Fourier transform of this characteristic function, the work probability distribution can be obtained. When the smearing function is spherically symmetric and the field is massless, it is

$$\begin{aligned}P(W) = (1-p)\delta(W) + \frac{\lambda^2}{2\pi}|\widetilde{\chi}(W)|^2|\widetilde{F}(W)|^2 W \\ \times\left(\frac{e^{\beta W}}{e^{\beta W}-1}\Theta(W) + \frac{1}{1-e^{-\beta W}}\Theta(-W)\right),\end{aligned} \tag{11}$$

where $p := \int_{W\neq 0}\mathrm{d}W P(W)$ and $\Theta(W)$ is the Heaviside function. Note that the case of the vacuum state of the field can be obtained by taking the well-defined limit $\beta\to\infty$ on Eq. (11).

In Fig. 1, we plot the work distribution for the unitary (8) (omitting the delta functions at the origin) acting on initial KMS states with $\beta = 1$ and $\beta\to\infty$ (the vacuum state) for a particular choice of the switching and smearing functions. As we can see in Fig. 1, unlike the case of the vacuum, there is a nonzero probability of the field doing work against the performer of the unitary, $W<0$. However, the probability of $W>0$ is larger than the probability of $W<0$, as granted by the second law. As the duration of the process goes to infinity, the probability distribution gets concentrated around zero and the negative part of the distribution vanishes, as expected in the quasi-static limit.

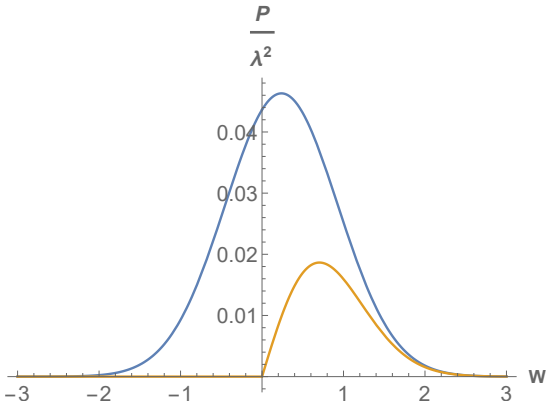

FIG. 1. Work distribution for the localized unitary acting on two KMS states: the vacuum ($\beta \to \infty$) and a state with $\beta = 1$. The switching and smearing functions are of the form $\chi(t) = \exp\left[-(t-\frac{T}{2})^2(T^2/72)^{-1}\right]$ and $F(\boldsymbol{x}) = \exp\left[-\frac{\boldsymbol{x}^2}{2\sigma^2}\right]$, with $T = \sigma = 1$. Note that the length of the interval $[0, T]$ is 12 times the standard deviation of the switching function.

Analysing the work distribution.- With the characteristic function $\widetilde{P}(\mu)$ now calculated, we can calculate the moments of $P(W)$ to gain some insight about the energy cost of applying a localized unitary to a quantum field. Since $\widetilde{P}(\mu) = \langle e^{\mathrm{i}\mu W}\rangle$, the k-th moment is

$$\langle W^k\rangle = \mathrm{i}^{-k}\frac{\mathrm{d}^k}{\mathrm{d}^k\mu}\widetilde{P}(\mu)|_{\mu=0}. \tag{12}$$

By using this and the expression for $\widetilde{P}(\mu)$ in (10), we obtain that the first and second order moments of the work distribution for the vacuum are:

$$\langle W\rangle = \lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2, \tag{13}$$

$$\langle W^2\rangle = \lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2\omega_{\boldsymbol{k}}. \tag{14}$$

From here we can obtain the variance $\sigma_W^2 = \langle W^2\rangle - \langle W\rangle^2 = \langle W^2\rangle + \mathcal{O}(\lambda^4)$.

An interesting observation is that, for the vacuum, if we consider unitaries that are very localized in time and space, both $\widetilde{\chi}(\omega_{\boldsymbol{k}})$ and $\widetilde{F}(\boldsymbol{k})$ will be wide in the frequency space, which means that the work variance will become larger than the expectation value, making the variance of the work increasingly significant as the operation on the field becomes increasingly localized in both time and space.

For an arbitrary KMS state of inverse temperature β, the value for $\langle W\rangle$ coincides with that of the vacuum (and $\langle W\rangle \geq 0$ as expected from the passivity of KMS states). In fact, since the imaginary part of the characteristic function does not depend on β, none of the odd-numbered moments will depend on temperature. For the variance, we have

$$\sigma_\beta^2 = \frac{\lambda^2}{2}\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\frac{e^{\beta\omega_{\boldsymbol{k}}}+1}{e^{\beta\omega_{\boldsymbol{k}}}-1}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2\omega_{\boldsymbol{k}} + \mathcal{O}(\lambda^4), \tag{15}$$

which shows that it monotonically increases with temperature.

We can also check that Crooks' theorem [24] is satisfied. The theorem states that for a process in which the Hamiltonian evolves from $\hat{H}(0) = \hat{H}_1$ to $H(T) = \hat{H}_2$, together with its time-reversed process, we have that

$$\frac{P(W)}{P_{\mathrm{rev}}(-W)} = e^{\beta W}\frac{Z_2}{Z_1}, \tag{16}$$

where Z_1, Z_2 are the partition functions of the thermal states of $\hat{H}(t_1)$ and $\hat{H}(t_2)$ and the initial state must be thermal in both processes, with the corresponding Hamiltonian.

In our example, we have, from equation (10) that $\widetilde{P}(\mu) = \widetilde{P}_{\mathrm{rev}}(-\mu + \mathrm{i}\beta)$, and since $\hat{H}(0) = \hat{H}(T) = \hat{H}_0$, $Z_2/Z_1 = 1$. Thus by taking the inverse Fourier transform we recover Eq.(16). Finally, the Jarzynski equality $\langle e^{-\beta W}\rangle = 1$, which is implied from the Crooks theorem, is satisfied. This can be seen just by evaluating the characteristic function at $\mu = \mathrm{i}\beta$.

Conclusion.- Conceptualizing the notion of work distributions for localized operations on quantum fields is challenging because a) energy eigenstates are not localized and b) projective measurements cannot be allowed in a relativistic quantum theory [8–10]. The two-projective measurement scheme employed in the literature [5] is hence ill-defined in QFT, but we have shown that one can still make sense of it via the Ramsey scheme that was designed to measure TPM work distributions [14, 15]. As such, we make a proposal of a well-defined work distribution in quantum field theory that, unlike [13], does not require the existence of projective measurements and does not inherit any complications from the fact that energy eigenstates are non-local. We have shown that this work distribution satisfies both the Jarzynski equality and Crooks' theorem for KMS states.

An interesting observation is that the work distribution that we define can be used to compute ratios of partition functions of field theories. Indeed we can invert the relationship (16) and write

$$\frac{Z_2}{Z_1} = e^{-\beta W}\frac{P(W)}{P_{\mathrm{rev}}(-W)}. \tag{17}$$

This can in fact be more simply obtained from Jarzynski's equality

$$\frac{Z_2}{Z_1} = \left\langle e^{-\beta W}\right\rangle. \tag{18}$$

Since computing work distributions with the proposed method is relatively simple, this potentially provides a

new way to compute these ratios, which are usually extremely difficult to calculate in QFT through path integral methods. The idea of calculating the ratio of partition functions from a non-equilibrium process has been used repeatedly in very different contexts (see e.g. [25–27] for applications in biochemistry).

With our framework, we have been able to obtain expressions for the work fluctuations associated to a process generated by a local Hamiltonian on a scalar field. We observe that the work fluctuations increase with temperature, and we show that the work fluctuations dominate the average work cost as the process becomes increasingly localized in both time and space. Also, we find that for KMS states of finite temperature, there is a non-zero probability of the field doing work when the process is of finite duration. It should be interesting to see how the work distribution relates to the variation of internal energy in the field in adiabatic and non-adiabatic processes. The internal energy of the field is given by the re-normalized stress-energy density, and exploring the connection between the stress-energy density deposited (or extracted) from the field and the work distributions of the processes where the energy is deposited can shed some light into the thermodynamics of local processes in quantum field theory.

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Details of the calculation of the state of the qubit

Field in the vacuum state

We now proceed to calculate the different terms of the perturbative expansion in (9). Clearly, $\hat{\rho}_T^{(0)} = \mathrm{Tr}_\phi\left(\hat{\rho}_0\right) = |+\rangle\langle+|$. It is easy to see that the first order term $\hat{\rho}_T^{(1)}$ will vanish. When taking the trace over the field, all the free evolution terms will end up multiplying the vacuum state, either at their left or at their right, so they will disappear, leaving $\langle\Omega|\,\hat{U}^{(1)}\,|\Omega\rangle$ or $\langle\Omega|\,\hat{U}^{\dagger(1)}\,|\Omega\rangle$. This is zero since

$$\hat{U}^{(1)} = -\mathrm{i}\lambda\int_{-\infty}^{\infty}\mathrm{d}t\int\mathrm{d}^3\boldsymbol{x}\chi(t)F(\boldsymbol{x})\hat{\phi}(t,\boldsymbol{x}), \tag{19}$$

and $\langle\Omega|\,\hat{\phi}(t,\boldsymbol{x})\,|\Omega\rangle = 0\ \forall\ t,\ \boldsymbol{x}$.

$\hat{\rho}_T^{(2)}$ is the sum of two contributions, one involving products with $\hat{U}^{(1)}$ and $\hat{U}^{\dagger(1)}$, and the other with $\hat{U}^{(2)}$. Let us focus on the first family of terms.

As an example, we explicitly calculate the coefficient associated to the component $\frac{|0\rangle\langle 0|}{2}$ of the density matrix of the qubit.

$$\begin{aligned}
\mathrm{Tr}\left(\hat{U}^{(1)}e^{-\mathrm{i}\mu\hat{H}_0}\,|\Omega\rangle\langle\Omega|\,e^{\mathrm{i}\mu\hat{H}_0}\hat{U}^{\dagger(1)}\right) &= \mathrm{Tr}\left(\hat{U}^{(1)}\,|\Omega\rangle\langle\Omega|\,\hat{U}^{\dagger(1)}\right)\\
&= \mathrm{Tr}\left(\lambda^2\int_{-\infty}^{\infty}\mathrm{d}t\chi(t)\int_{-\infty}^{\infty}\mathrm{d}t'\chi(t')\int\mathrm{d}^3\boldsymbol{x}F(\boldsymbol{x})\int\mathrm{d}^3\boldsymbol{x}'F(\boldsymbol{x}')\hat{\phi}(t,\boldsymbol{x})\,|\Omega\rangle\langle\Omega|\,\hat{\phi}(t',\boldsymbol{x}')\right)\\
&= \mathrm{Tr}\left(\lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}'}{(2\pi)^3\sqrt{2\omega_{\boldsymbol{k}}}\sqrt{2\omega_{\boldsymbol{k}'}}}\int_{-\infty}^{\infty}\mathrm{d}t\chi(t)e^{i\omega_{\boldsymbol{k}}t}\int\mathrm{d}^3\boldsymbol{x}F(\boldsymbol{x})e^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}}\right.\\
&\qquad\left.\times\int_{-\infty}^{\infty}\mathrm{d}t'\chi(t')e^{-\mathrm{i}\omega_{\boldsymbol{k}'}t'}\int\mathrm{d}^3\boldsymbol{x}'F(\boldsymbol{x}')e^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{x}'}|\boldsymbol{k}\rangle\langle\boldsymbol{k}'|\right)\\
&= \lambda^2\,\mathrm{Tr}\left(\int\frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}^3\boldsymbol{k}'}{(2\pi)^3\sqrt{2\omega_{\boldsymbol{k}}}\sqrt{2\omega_{\boldsymbol{k}'}}}\widetilde{\chi}(\omega_{\boldsymbol{k}})\widetilde{\chi}(-\omega_{\boldsymbol{k}'})\widetilde{F}(-\boldsymbol{k})\widetilde{F}(-\boldsymbol{k}')|\boldsymbol{k}\rangle\langle\boldsymbol{k}'|\right)\\
&= \lambda^2\int\frac{\mathrm{d}^3k}{(2\pi)^3 2\omega_{\boldsymbol{k}}}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2,
\end{aligned} \tag{20}$$

where in the last step we have used that $FT[f](x) = (FT[f](-x))^*$, for a real function f. We are assuming that both the switching and the smearing are real functions. The calculation for the $\frac{|1\rangle\langle 0|}{2}$ coefficient is analogous, the

only difference being the presence of a factor $e^{-i\mu\hat{H}_0}$ multiplying the ket vectors $|\boldsymbol{k}\rangle$. Since $e^{-\mathrm{i}\mu\hat{H}_0}|\boldsymbol{k}\rangle = e^{-\mathrm{i}\mu\omega_{\boldsymbol{k}}}|\boldsymbol{k}\rangle$, we obtain that

$$\mathrm{Tr}\left(e^{-\mathrm{i}\mu\hat{H}_0}\hat{U}^{(1)}\left|\Omega\right\rangle\left\langle\Omega\right|e^{\mathrm{i}\mu\hat{H}_0}\hat{U}^{\dagger(1)}\right) = \lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2 e^{-\mathrm{i}\mu\omega_{\boldsymbol{k}}}. \tag{21}$$

The rest of the components are the Hermitian conjugates of these.

We now calculate the remaining terms. That is, the terms that involve products with $\hat{U}^{(2)}$. Let us start by obtaining $\mathrm{Tr}_\phi\left(\hat{U}^{(2)}e^{-\mathrm{i}\mu\hat{H}_0}\left|\Omega\right\rangle\left\langle\Omega\right|e^{\mathrm{i}\mu\hat{H}_0}\otimes\frac{|0\rangle\langle 0|}{2}+H.c\right) = \left\langle\Omega\right|\hat{U}^{(2)}\left|\Omega\right\rangle\frac{|0\rangle\langle 0|}{2}+H.c.$ This is simply

$$\begin{aligned}-\lambda^2\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{t}\mathrm{d}t'\int\mathrm{d}^3\boldsymbol{x}\int\mathrm{d}^3\boldsymbol{x}'\chi(t)\chi(t')F(\boldsymbol{x})F(\boldsymbol{x}')\left\langle\Omega\right|\hat{\phi}(t,\boldsymbol{x})\hat{\phi}(t',\boldsymbol{x}')\left|\Omega\right\rangle\frac{|0\rangle\langle 0|}{2}+H.c \\ = -\lambda^2\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{t}\mathrm{d}t'\int\mathrm{d}^3\boldsymbol{x}\int\mathrm{d}^3\boldsymbol{x}'\chi(t)\chi(t')F(\boldsymbol{x})F(\boldsymbol{x}')2\,\mathrm{Re}[\mathcal{W}(t,\boldsymbol{x},t',\boldsymbol{x}')]\frac{|0\rangle\langle 0|}{2},\end{aligned} \tag{22}$$

where $\mathcal{W}(t,\boldsymbol{x},t',\boldsymbol{x}') = \left\langle\Omega\right|\hat{\phi}(t,\boldsymbol{x})\hat{\phi}(t',\boldsymbol{x}')\left|\Omega\right\rangle$ is the Wightman function. The same is obtained for the other cases. This is because all the $e^{\pm i\mu\hat{H}_0}$ end up multiplying the vacuum state when taking the trace, so they disappear leaving simply $\left\langle\Omega\right|\hat{U}^{(2)}\left|\Omega\right\rangle + H.c.$ Therefore, the contribution of these terms to the reduced state of the qubit is $A\left|+\right\rangle\left\langle+\right|$, where

$$A = -\lambda^2\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{t}\mathrm{d}t'\int\mathrm{d}^3\boldsymbol{x}\int\mathrm{d}^3\boldsymbol{x}'\chi(t)\chi(t')F(\boldsymbol{x})F(\boldsymbol{x}')2\,\mathrm{Re}[\mathcal{W}(t,\boldsymbol{x},t',\boldsymbol{x}')]. \tag{23}$$

Adding everything and noting that (20) is equal to (23) we obtain, after applying the second Hadamard on the qubit, that the reduced state can be written as

$$\hat{\rho}_\mu = \frac{1}{2}\left(\mathbb{I} + \left|-\right\rangle\left\langle+\right|\left(1+\lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2\left(e^{-\mathrm{i}\mu\omega_{\boldsymbol{k}}}-1\right)\right)\right. \tag{24}$$

$$\left. + \left|+\right\rangle\left\langle-\right|\left(1+\lambda^2\int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}}|\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2|\widetilde{F}(\boldsymbol{k})|^2\left(e^{\mathrm{i}\mu\omega_{\boldsymbol{k}}}-1\right)\right)\right). \tag{25}$$

Field in a finite-temperature KMS state

Some properties that we use throughout these calculation are:

$$\mathrm{Tr}\left(\hat{\phi}\hat{\rho}_\beta\right) = 0, \tag{26}$$

$$\left[\hat{\rho}_\beta, e^{-it\hat{H}_0}\right] = 0. \tag{27}$$

As before, we calculate the reduced state of the qubit with a Dyson expansion. The first order term is again zero. As an example of why this is the case, we calculate

$$\mathrm{Tr}\left(e^{-\mathrm{i}\mu\hat{H}_0}\hat{U}^{(1)}\hat{\rho}_\beta e^{\mathrm{i}\mu\hat{H}_0}\right) + \mathrm{Tr}\left(e^{-\mathrm{i}\mu\hat{H}_0}\hat{\rho}_\beta e^{\mathrm{i}\mu\hat{H}_0}\hat{U}^{\dagger(1)}\right) = \mathrm{Tr}\left(\hat{U}^{(1)}\hat{\rho}_\beta\right) + Tr\left(\hat{\rho}_\beta\hat{U}^{\dagger(1)}\right), \tag{28}$$

where we have used the cyclic property of the trace and (27). Finally, using the linearity of the trace, the expression for $\hat{U}^{(1)}$ and (26), we obtain that both terms are zero. A similar procedure can be used to check that all the other contributions to the first order correction are zero.

We now calculate the second order terms, starting by the ones that only involve products of $\hat{U}^{(1)}$ and $\hat{U}^{\dagger(1)}$. We derive here only the coefficient of $\frac{|0\rangle\langle 1|}{2}$. The other cases follow analogously.

$$\mathrm{Tr}\left(\hat{U}^{(1)}e^{-\mathrm{i}\mu\hat{H}_0}\hat{\rho}_\beta\hat{U}^{\dagger(1)}e^{\mathrm{i}\mu\hat{H}_0}\right) = \mathrm{Tr}\left(e^{\mathrm{i}\mu\hat{H}_0}\hat{U}^{(1)}e^{-\mathrm{i}\mu\hat{H}_0}\hat{\rho}_\beta\hat{U}^{\dagger(1)}\right). \tag{29}$$

We have that

$$\begin{aligned}e^{\mathrm{i}\mu\hat{H}_0}\hat{U}^{(1)}e^{-\mathrm{i}\mu\hat{H}_0} &= -\mathrm{i}\lambda\int_{-\infty}^{\infty}\mathrm{d}t\int\mathrm{d}^3\boldsymbol{x}\chi(t)F(\boldsymbol{x})e^{\mathrm{i}\mu\hat{H}_0}\hat{\phi}(\boldsymbol{x},t)e^{-\mathrm{i}\mu\hat{H}_0} \\ &= -\mathrm{i}\lambda\int_{-\infty}^{\infty}\mathrm{d}t\int\mathrm{d}^3\boldsymbol{x}\chi(t)F(\boldsymbol{x})\hat{\phi}(\boldsymbol{x},t+\mu).\end{aligned} \tag{30}$$

So (29) equals

$$\lambda^2 \int \mathrm{d}t \int \mathrm{d}t' \int \mathrm{d}^3\boldsymbol{x} \int \mathrm{d}^3\boldsymbol{x}' \chi(t)\chi(t') F(\boldsymbol{x})F(\boldsymbol{x}') \operatorname{Tr}\left(\hat{\phi}(\boldsymbol{x}, t+\mu)\hat{\rho}_\beta \hat{\phi}(\boldsymbol{x}', t'+\mu)\right) \tag{31}$$
$$= \lambda^2 \int \mathrm{d}t \int \mathrm{d}t' \int \mathrm{d}^3\boldsymbol{x} \int \mathrm{d}^3\boldsymbol{x}' \chi(t)\chi(t') F(\boldsymbol{x})F(\boldsymbol{x}') \mathcal{W}_\beta(\boldsymbol{x}', t', \boldsymbol{x}, t+\mu).$$

The other terms have the same structure, with the only change being in the thermal Wightman function, which is $\mathcal{W}(x', t', x, t)$ for the diagonal terms, and $\mathcal{W}(x', t', x, t-\mu)$ for the $\frac{|1\rangle\langle 0|}{2}$ term.

Let us obtain now the second order terms coming from products with $\hat{U}^{(2)}$ and $\hat{U}^{\dagger(2)}$. It is easy to see, using (27) that all the terms are equal to

$$\operatorname{Tr}\left(\hat{U}^{(2)}\hat{\rho}_\beta\right) + \operatorname{Tr}\left(\hat{\rho}_\beta \hat{U}^{\dagger(2)}\right) = 2\operatorname{Re}\operatorname{Tr}\left(\hat{U}^{(2)}\hat{\rho}_\beta\right). \tag{32}$$

This finishes the proof. Since the Dyson expansion preserves the trace of the density matrix, Eq. (31) has to be equal to Eq. (32), so as to cancel the diagonals added by the perturbation terms. This is useful because it gives a much more compact expression for the reduced state of the qubit. Therefore, at the end of the Ramsey scheme, the density matrix of the qubit is:

$$\frac{1}{2}\left(\mathbb{I} + |+\rangle\langle -| \left(1 + \lambda^2 \int \mathrm{d}t \int \mathrm{d}t' \int \mathrm{d}^3\boldsymbol{x} \int \mathrm{d}^3\boldsymbol{x}' \chi(t)\chi(t') F(\boldsymbol{x})F(\boldsymbol{x}') \left(\mathcal{W}_\beta(\boldsymbol{x}', t', \boldsymbol{x}, t+\mu) - \mathcal{W}_\beta(\boldsymbol{x}', t', \boldsymbol{x}, t)\right)\right)\right. \tag{33}$$
$$\left. + |-\rangle\langle +| \left(1 + \lambda^2 \left(\int \mathrm{d}t \int \mathrm{d}t' \int \mathrm{d}^3\boldsymbol{x} \int \mathrm{d}^3\boldsymbol{x}' \chi(t)\chi(t') F(\boldsymbol{x})F(\boldsymbol{x}') \left(\mathcal{W}_\beta(\boldsymbol{x}', t', \boldsymbol{x}, t-\mu) - \mathcal{W}_\beta(\boldsymbol{x}', t', \boldsymbol{x}, t)\right)\right)\right)\right).$$

Using the expression of the Wightman function for a thermal state of inverse temperature β [23]

$$\mathcal{W}_\beta(\boldsymbol{x}', t', \boldsymbol{x}, t) = \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}} \left(e^{\beta\omega_{\boldsymbol{k}}} - 1\right)} \left(e^{\beta\omega_{\boldsymbol{k}}} e^{\mathrm{i}k(\boldsymbol{x}-\boldsymbol{x}')} + e^{\mathrm{i}k(\boldsymbol{x}'-\boldsymbol{x})}\right), \tag{34}$$

we can calculate the characteristic function of the work distribution

$$\widetilde{P}(\mu) = 1 + \lambda^2 \int \frac{d^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}} \left(e^{\beta\omega_{\boldsymbol{k}}} - 1\right)} |\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2 |\widetilde{F}(\boldsymbol{k})|^2 \left(e^{\beta\omega_{\boldsymbol{k}}} + 1\right) \left(\cos(\mu\omega_{\boldsymbol{k}}) - 1\right) \tag{35}$$
$$+ \mathrm{i}\lambda^2 \int \frac{d^3\boldsymbol{k}}{(2\pi)^3 2\omega_{\boldsymbol{k}}} |\widetilde{\chi}(\omega_{\boldsymbol{k}})|^2 |\widetilde{F}(\boldsymbol{k})|^2 \sin(\mu\omega_{\boldsymbol{k}}).$$

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