Lectures on quantum fields and information theory

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ABSTRACT: Notes for four lectures that introduce students of physics to information theoretic aspects of quantum field theory. Prepared for a course at Heidelberg university in the summer term 2018.

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1 Entropy as a measure of information

1.1 Shannon's information entropy

To a set of measurement outcomes, or more general realizations of a random variable, one can associate symbols $\{x_1, \ldots, x_N\}$ and probabilities

$$p(x_1), \dots, p(x_N). \tag{1.1}$$

Of course one has

$$1 = p(x_1) + \ldots + p(x_N) = \sum_{x} p(x).$$
 (1.2)

The last equation introduces a short hand notation we will use occasionally.

For two events X and Y with possible outcomes $\{x_m\}$ and $\{y_n\}$ one has a complete description in terms of *joint probabilities*

$$p(x_m, y_n), (1.3)$$

such that $1 = \sum_{x,y} p(x,y)$. One should read the comma as "and". If the two events are *statistically independent* one has

$$p(x,y) = p(x)p(y), (1.4)$$

but that is of course not always the case. More general, the reduced probabilities for one event are

$$p(x) = \sum_{y} p(x, y),$$
 $p(y) = \sum_{x} p(x, y).$ (1.5)

Assume now that one has already learned the outcome x_0 , then the new probability distribution for y is

$$p(y_n|x_0) = \frac{p(x_0, y_n)}{\sum_k p(x_0, y_k)} = \frac{p(x_0, y_n)}{p(x_0)},$$
(1.6)

which is the *conditional probability*. (Read: probability for y_n under the condition that x_0 has been obtained.) One can write

$$p(x_m, y_n) = p(y_n | x_m) p(x_m) = p(x_m | y_n) p(y_n),$$
(1.7)

which directly implies Bayes' theorem.

$$p(x_m|y_n) = \frac{p(y_n|x_m) p(x_m)}{p(y_n)}.$$
(1.8)

How much information can one learn from an outcome or event realization x? Or, in other words, how large is the information content i(x) associated with the outcome x? Intuitively, the less likely the outcome, the higher the information content. Moreover, for independent events it is natural to take the information content additive,

$$i(p(x,y)) = i(p(x)p(y)) = i(p(x)) + i(p(y)).$$
(1.9)

This directly leads to the logarithm, and the definition of the information content

$$i(x) = i(p(x)) = -\ln p(x).$$
 (1.10)

In principle one might add a (positive) prefactor here or, equivalently, take another base for the logarithm. Oftentimes \log_2 is used, but we work here with the natural logarithm. For example, throwing an ideal coin corresponds to $p(x_1) = p(x_2) = 1/2$ and by learning the event outcome one learns an amount of information

$$i = -\ln(1/2) = \ln 2,\tag{1.11}$$

corresponding to one bit of information. Note that a very unlikely event outcome with $p \to 0$ has formally infinite information content, $i \to \infty$. On the other side, a certain event outcome with unit probability, p = 1, has no information content, i = 0.

Shannon's information entropy associated to a discrete random variable or event X is the expected amount of information content,

$$H(X) = \langle i(x) \rangle = -\sum_{x} p(x) \ln p(x). \tag{1.12}$$

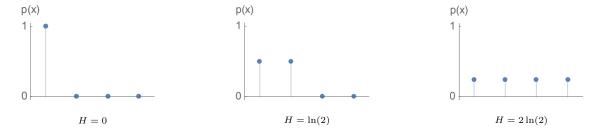


Figure 1: Examples for discrete probability distributions and associated information entropy H.

Note that the information entropy is a functional of the probability distribution only, H(X) = H[p(x)]. For some examples of discrete probability distributions and associated information entropy, see figure 1.

Some properties of information entropy are

- i) Non-negativity. Information entropy for discrete random variables is positive semi-definite, $H(X) \ge 0$.
- ii) Concavity. Define a random variable X with probability distribution p(x) out of distributions $p_A(x)$ and $p_B(x)$ for the variables X_A and X_B such that

$$p(x) = q p_A(x) + (1 - q) p_B(x). (1.13)$$

One has then

$$H(X) \ge qH(X_A) + (1-q)H(X_B).$$
 (1.14)

Exercise: Show this property.

- iii) Permutation invariance. If one relabels the event outcomes by some permutation of indices $x_m \to x_{\pi(m)}$, the information entropy is unchanged. This is directly clear from the definition.
- iv) Minimum value. One has H(X) = 0 if and only if X is deterministic such that p(x) = 1 for one outcome x.
- v) Maximum value. For a set of event outcomes of size or cardinality |X| one has

$$H(X) \le \ln|X|. \tag{1.15}$$

Proof: maximize the probability distribution p(x) with the condition that it remains normalized. This corresponds to finding the extremum of

$$\mathcal{L} = H(X) + \lambda \left(\sum_{x} p(x) - 1 \right). \tag{1.16}$$

One has

$$\frac{\partial \mathcal{L}}{\partial p(x)} = -\ln p(x) - 1 + \lambda = 0 \qquad \Rightarrow \qquad p(x) = e^{\lambda - 1}. \tag{1.17}$$

This depends only on λ but must be normalized. Normalization leads to p(x) = 1/|X| and $H(X) = \ln |X|$.

1.2 Conditional entropy

If two variables are correlated they are not statistically independent. One may say that Y contains side information about X. Define the *conditional information content* via the conditional probability

$$i(x|y) = -\ln p(x|y). \tag{1.18}$$

The conditional entropy is defined as the following expectation value of the conditional information content,

$$H(X|Y) = -\sum_{x,y} p(x,y) \ln p(x|y). \tag{1.19}$$

This can be seen as the expected information content of surprise when learning an outcome x after already knowing the outcome y. One can show the following: Conditioning does not increase entropy,

$$H(X) \ge H(X|Y). \tag{1.20}$$

Here H(X) is the information entropy corresponding to the reduced probability p(x). The proof will be given further below.

1.3 Joint entropy

The joint entropy is simply the entropy associated with the joint probability distribution

$$H(X,Y) = -\sum_{x,y} p(x,y) \ln p(x,y).$$
 (1.21)

Exercise: Verify that H(X,Y) = H(X) + H(Y|X) = H(Y) + H(X|Y).

1.4 Mutual information

The mutual information of two random variables X and Y is the entropy of one variable less the conditional entropy,

$$I(X;Y) = H(X) - H(X|Y). (1.22)$$

It corresponds to the expected gain in information (or loss of uncertainty) about the variable X when learning an event outcome y of the random variable Y. One can express the mutual information also as

$$I(X;Y) = \sum_{x,y} p(x,y) \ln \left(\frac{p(x,y)}{p(x)p(y)} \right). \tag{1.23}$$

This makes the symmetry I(X;Y) = I(Y;X) manifest. One can therefore also write

$$I(X;Y) = H(Y) - H(Y|X). (1.24)$$

Note that the statement conditioning does not increase entropy is equivalent to

$$I(X;Y) \ge 0, (1.25)$$

which will be proven below. In fact, one has I(X;Y) = 0 if and only if X and Y are independent random variables such that p(x,y) = p(x)p(y).

1.5 Relative entropy (or Kullback-Leibler divergence)

The relative entropy is a useful quantity to compare two probability distributions p(x) and q(x). It is defined by

$$D(p||q) = \sum_{x} p(x) \left[\ln p(x) - \ln q(x) \right]. \tag{1.26}$$

This definition works if the support of the function p(x) (the set of values x where p(x) > 0) is within the support of the function q(x). In that case there are no points where p(x) > 0 but q(x) = 0. For cases where this condition is not fulfilled, one can extend the definition of relative entropy in a natural way to $D(p||q) = \infty$. Note that one can write the relative entropy as an expectation value with respect to the probability distribution p(x),

$$D(p||q) = \left\langle \ln \left(\frac{p(x)}{q(x)} \right) \right\rangle_{p}. \tag{1.27}$$

The relative entropy tells in some sense how far the distribution function p(x) is from the distribution function q(x). However, it is not defined symmetrically (nor does it satisfy a triangle inequality) and is therefore not a distance measure or metric in the mathematical sense.

Typically, relative entropy is used to compare two probability distributions where p(x) is often the true distribution and q(x) some kind of approximation to it. It then has the meaning of a gain in information when one replaces the (approximate) model distribution q(x) by the true (or more accurate) distribution p(x). It can also denote a loss of information, or added uncertainty, if one works with q(x) instead of p(x).

To illustrate the asymmetry in the definition, consider the following two examples.

i) Take $p(x_1) = 1$ and $p(x_2) = p(x_3) = \ldots = 0$ and compare this to $q(x_1) = 1 - \epsilon$, $q(x_2) = \epsilon$ and $q(x_3) = \ldots = q(x_N) = 0$. One has

$$D(p||q) = -\ln(1 - \epsilon) \approx \epsilon. \tag{1.28}$$

The gain in knowledge from q(x) to p(x) is moderate and vanishes for $\epsilon \to 0$ because q(x) is already very close to p(x) on all outcomes x allowed by the true probability distribution p(x) (i. e. on x_1). An experiment that has been designed in an optimal way based on the (wrong) prior distribution q(x) will nevertheless find the correct distribution p(x) rather efficiently.

ii) Take instead $p(x_1)=1-\epsilon$, $p(x_2)=\epsilon$ and $p(x_3)=\ldots=p(x_N)=0$ and compare this to $q(x_1)=1$ and $q(x_2)=\ldots=q(x_N)=0$. One has now formally

$$D(p||q) = (1 - \epsilon) \ln\left(\frac{1 - \epsilon}{1}\right) + \epsilon \ln\left(\frac{\epsilon}{0}\right) = \infty.$$
 (1.29)

Here the gain in information when replacing the model distribution q(x) by the true distribution p(x) is much larger. The model distribution q(x) vanishes on the state x_2 which has actually non-vanishing probability according to p(x). It is very difficult to find out about this and one needs formally infinitely good statistics in an experiment that is optimized based on the prior distribution q(x) (assuming misguidedly that x_2 is never realized).

An important property of relative entropy is its non-negativity,

$$D(p||q) \ge 0. \tag{1.30}$$

This follows from the inequality $ln(x) \le x - 1$. One sees directly

$$D(p||q) = \sum_{x} p(x) \ln\left(\frac{p(x)}{q(x)}\right) = -\sum_{x} p(x) \ln\left(\frac{q(x)}{p(x)}\right) \ge \sum_{x} p(x) \left(1 - \frac{q(x)}{p(x)}\right) = 0. \tag{1.31}$$

Note also that mutual information can be written as a relative entropy,

$$I(X;Y) = D(p(x,y)||p(x)p(y)), (1.32)$$

so it can be seen as the information gained when one learns that the true distribution is p(x, y) and not the factorized distribution p(x)p(y). Note also that positivity of relative entropy directly implies positivity of mutual information which in turn implies the statement *conditioning does not increase entropy*. This completes the proofs left open above.

Relative entropy has the advantage that it generalizes favorably to continuous probability distributions. Consider the continuum limit

$$p(x_m) \to \mathcal{P}(x)dx, \qquad q(x_m) \to \mathcal{Q}(x)dx,$$
 (1.33)

with probability densities $\mathcal{P}(x)$ and $\mathcal{Q}(x)$. The relative entropy becomes

$$D(p||q) = \int dx \, \mathcal{P}(x) \left[\ln(\mathcal{P}(x)dx) - \ln(\mathcal{Q}(x)dx) \right] = \int dx \, \mathcal{P}(x) \left[\ln \mathcal{P}(x) - \ln \mathcal{Q}(x) \right]. \tag{1.34}$$

In contrast, Shannon's entropy has the formal continuum limit

$$H(X) \to \int dx \, \mathcal{P}(x) \ln(\mathcal{P}(x)dx),$$
 (1.35)

which is not very well defined.

1.6 Fisher information metric

The relative entropy is positive semi-definite and one has D(p||q) = 0 if and only if p(x) = q(x). However, it is not a distance measure in the mathematical sense because it is not symmetric, $D(p||q) \neq D(q||p)$. In the limit where p and q are very close, it satisfies the properties of a metric, however. To make this more precise, consider a set of probability distributions $p(\theta)(x)$ where θ is a (multi-dimensional) parameter. Close to some point θ_0 one may expand

$$D(p(\theta)||p(\theta_0)) = \frac{1}{2}(\theta^j - \theta_0^j)(\theta^k - \theta_0^k)g_{jk}(\theta_0) + \dots$$
 (1.36)

The constant and linear terms vanish because D(p||q) is positive semi-definite and vanishes at p=q. The object $g_{jk}(\theta_0)$ is known as the Fisher information metric. It is by construction symmetric and serves as a Euclidean, positive semi-definite metric on the space of parameters θ of probability distributions $p(\theta)$. One may also see this as a two-form constructed via the pull-back of the map $\theta \to p(\theta)$ from a metric directly defined on the space of probability functions. The latter is obtained from the expansion

$$D(q + \delta q || q) = \sum_{x} \frac{1}{2q(x)} \delta q(x)^{2} + \dots$$
 (1.37)

We have set here $p(x)=q(x)+\delta q(x)$ and used that both p and q are normalized such that $\sum_x \delta q(x)=0$.

1.7 von Neumann's quantum entropy

The quantum entropy or von Neumann entropy is defined for a given quantum density matrix (or density operator) ρ as

$$S(\rho) = -\operatorname{tr}\left\{\rho \ln \rho\right\}. \tag{1.38}$$

The logarithm of an operator is here defined via its eigenvalues. Recall that $\rho = \rho^{\dagger}$ is hermitean and can always be diagonalized such that it has the form

$$\rho = p_j |j\rangle\langle j|,\tag{1.39}$$

where the states $|j\rangle$ are orthogonal and normalized, $\langle j|k\rangle = \delta_{jk}$. In this basis one has

$$S(\rho) = -\sum_{j} p_j \ln p_j = H(p)$$
(1.40)

with Shannon entropy H. The quantum entropy has the properties

i) Non-negativity.

$$S(\rho) \ge 0. \tag{1.41}$$

This follows from the fact that the density matrix has eigenvalues in the range $0 \le p_j \le 1$. Of course, $S(\rho) = 0$ for a pure state $\rho = |\psi\rangle\langle\psi|$ while mixed states have S > 0.

- ii) Maximum value. Occurs for maximally mixed states. In an N-dimensional Hilbert space this corresponds to $\rho = \text{diag}(1/N)$ and $S(\rho) = \ln N$.
- iii) Invariance under unitary transformations. The density operator transforms as

$$\rho \to U \rho U^{\dagger},$$
 (1.42)

and the von Neumann entropy is invariant,

$$S(U\rho U^{\dagger}) = S(\rho). \tag{1.43}$$

This is immediately clear because unitary transformations due not change the eigenvalues.

1.8 Quantum relative entropy

The quantum version of relative entropy is defined for two normalized density matrices ρ and σ by

$$S(\rho||\sigma) = \operatorname{tr}\left\{\rho\left[\ln\rho - \ln\sigma\right]\right\}. \tag{1.44}$$

As in the classical case, this holds for $\sup(\rho) \subseteq \sup(\sigma)$ and is extended naturally by setting $S(\rho||\sigma)$ otherwise. Quantum relative entropy has rather useful properties and should presumably be used more often in quantum field theory.

1.9 Rényi entropy

The quantum Rényi entropy is defined for a parameter N > 0 (not necessarily integer) by

$$S_N(\rho) = \frac{1}{1 - N} \ln \operatorname{tr} \left\{ \rho^N \right\}. \tag{1.45}$$

As a special case, for $N \to 1$ the Rényi entropy becomes von Neumanns entropy [9, 10],

$$S_{N}(\rho) = \frac{1}{1 - N} \ln \operatorname{tr} \left\{ e^{N \ln \rho} \right\} = \frac{1}{1 - N} \ln \operatorname{tr} \left\{ \rho \left(1 + (N - 1) \ln \rho + \ldots \right) \right\}$$

$$\stackrel{N \to 1}{\to} -\operatorname{tr} \left\{ \rho \ln \rho \right\} = S(\rho).$$
(1.46)

One can sometimes calculate the Rényi entropy for arbitrary integer values $N \geq 2$ and determine the von Neumann entropy via analytic continuation $N \to 1$.

Note that for N=2 one has simply

$$S_2(\rho) = -\ln \operatorname{tr}\left\{\rho^2\right\}. \tag{1.47}$$

This is often a relatively simple quantity to compute (or measure experimentally) and allows to distinguish pure states with $S_2 = 0$ from mixed states with $S_2 > 0$.

One can also define a generalization of relative entropy in a similar way, the quantum $R\acute{e}nyi$ relative entropy

$$S_N(\rho||\sigma) = \frac{1}{N-1} \ln \frac{\text{tr}\{\rho\sigma^{N-1}\}}{\text{tr}\{\rho^N\}} = \frac{1}{N-1} \ln \text{tr}\{\rho\sigma^{N-1}\} - S_N(\rho).$$
 (1.48)

In the limit $N \to 1$ the quantum Rényi relative entropy approaches the quantum relative entropy, $S_N(\rho||\sigma) \stackrel{N \to 1}{\to} S(\rho||\sigma)$. Exercise: verify this.

1.10 Joint quantum entropy

The density operator of a composite system A + B is ρ_{AB} and has the joint entropy

$$S(\rho_{AB}) = -\operatorname{tr}\left\{\rho_{AB}\ln\rho_{AB}\right\},\tag{1.49}$$

where the trace goes over both systems, $tr = tr_A tr_B$. If there is no doubt, we will denote the full density matrix simply as $\rho_{AB} = \rho$ and the joint entropy as $S(\rho)$.

1.11 Entanglement entropy

The reduced density matrix for subsystem A of the full system A + B is defined by

$$\rho_A = \operatorname{tr}_B\{\rho\}. \tag{1.50}$$

The associated von Neumann entropy is also known as the entanglement entropy

$$S_A = -\operatorname{tr}_A \left\{ \rho_A \ln \rho_A \right\}. \tag{1.51}$$

In a similar way, the reduced density matrix for system B is $\rho_B = \operatorname{tr}_A\{\rho\}$ and the associated entropy is $S_B = -\operatorname{tr}_B\{\rho_B \ln \rho_B\}$.

For a pure state $\rho = |\phi\rangle\langle\phi|$ one can write in the Schmidt basis

$$|\phi\rangle = \sum_{i} \sqrt{\lambda_j} |j_A\rangle |j_B\rangle,$$
 (1.52)

where $\lambda_j \geq 0$ and $\sum_j \lambda_j = 1$. The reduced density matrices are

$$\rho_A = \sum_j \lambda_j |j_A\rangle\langle j_A|,$$

$$\rho_B = \sum_j \lambda_j |j_B\rangle\langle j_B|.$$
(1.53)

One has then for the entanglement entropy

$$S_A = S_B = -\sum_j \lambda_j \ln \lambda_j, \tag{1.54}$$

and in particular both entropies are equal. (This is not necessarily the case for mixed states $\rho \neq |\phi\rangle\langle\phi|$.) For a product state, only one coefficient $\lambda_0 = 1$ is non-vanishing and $S_A = S_B = 0$. Entangled states have several non-vanishing Schmidt basis coefficients and in this sense $S_A = S_B > 0$ is here a measure for the amount of entanglement between subsystems A and B.

2 Entropies and entanglement of Gaussian states

2.1 Quantum field theory

We adopt now a quantum field theoretic point of view and investigate concepts like entropy and entanglement in a field theoretic setup. Conceptually, quantum field theory can be understood as quantum mechanics with infinitely many degrees of freedom, for a bosonic theory for example one has one (or several) continuous degrees of freedom for each point in space. Let us consider a hypersurface of Minkowski space such as a plane (actually a three-volume) of constant time t, or more general any space-like Cauchy surface Σ . We assume that we have coordinates \mathbf{x} on the surface Σ . The degrees of freedom of the field theory correspond then to the field values

$$\phi_i(\mathbf{x}).$$
 (2.1)

We have here (at least) two type of "indices": one is the position \mathbf{x} , the other an additional discrete index j that could label different components. There might for example be an "internal" O(N) symmetry or we have complex fields such that $\phi_1(\mathbf{x}) = \varphi(\mathbf{x})$ and $\phi_2(\mathbf{x}) = \varphi^*(\mathbf{x})$, or there might be space-time indices if we consider vector or tensor fields, different flavors, and so on.

It will be useful in the following to combine all possible indices into one "abstract index"

$$m = (j, \mathbf{x}). \tag{2.2}$$

If we write \sum_m we mean then actually an appropriate combination of summations and integrations over the different indices. Note that this works equally well in position space as after a Fourier transform in spatial momentum space, at least in flat space and for a t= const hypersurface. Momentum is then just another basis to label and expand field configurations. For complex fields, we will also take their complex conjugate to be part of the "Nambu field" ϕ_m . Nevertheless, it will often be convenient to also talk about the complex conjugate field ϕ_m^* although it is not independent of ϕ_m .

Quantum states of the field theory on a hypersurface Σ can be conveniently expanded in the analog of the position space eigenfunctions in quantum mechanics. These are eigenstates of the field value operator

$$\Phi_m |\phi\rangle = \phi_m |\phi\rangle, \tag{2.3}$$

with eigenvalues ϕ_m . If the quantum system is in a pure state $|\Psi\rangle$, then $\langle \phi | \Psi \rangle = \Psi[\phi]$ represents its Schrödinger wave functional, to be understood as a functional of the field ϕ and to be seen as the analog of the Schrödinger wave function $\langle \mathbf{x} | \psi \rangle = \psi(\mathbf{x})$.

In principle, for arbitrary states in a quantum field theory, the Schrödinger functional can be a rather complicated object. I will concentrate here on an important subclass of states that have a Gaussian density matrix. This class contains vacuum and thermal states of non-interacting quantum field theories or perturbative extensions thereof, coherent states, squeezed states, and many more. However, it is clear that we make a restriction here. For conformal field theories we will later also go beyond the Gaussian case.

2.2 Gaussian pure states

The most general form of a Gaussian Schrödinger wave functional representing a pure state for a bosonic field theory can be written as

$$\langle \phi | \Psi \rangle = \exp \left[-\frac{1}{2} \phi_m^* h_{mn} \phi_n + \frac{i}{2} \phi_m^* \lambda_m + \frac{i}{2} \lambda_m^* \phi_m + \frac{1}{2} \phi_m^* \kappa_m + \frac{1}{2} \kappa_m^* \phi_m \right]$$

$$= \exp \left[-\frac{1}{2} \phi^{\dagger} h \phi + \frac{i}{2} \phi^{\dagger} \lambda + \frac{i}{2} \lambda^{\dagger} \phi + \frac{1}{2} \phi^{\dagger} \kappa + \frac{1}{2} \kappa^{\dagger} \phi \right].$$
(2.4)

¹For instance, in the absence of any other components, we have $\phi_1 = \phi$ and $\phi_2 = \phi^*$.

In the second equation, we have used a condensed notation with ϕ denotes the collection of fields, and h, λ and κ are complex quantities that parametrize the state. Their physical meaning will be discussed below. Gaussianity refers to the maximum power of the field appearing in the exponential (2.4) being quadratic. Correspondingly, we have

$$\langle \Psi | \phi \rangle = \exp \left[-\frac{1}{2} \phi^{\dagger} h^{\dagger} \phi - \frac{i}{2} \phi^{\dagger} \lambda - \frac{i}{2} \lambda^{\dagger} \phi + \frac{1}{2} \phi^{\dagger} \kappa + \frac{1}{2} \kappa^{\dagger} \phi \right]. \tag{2.5}$$

The norm is given by a functional integral over ϕ ,

$$\langle \Psi | \Psi \rangle = \int D\phi \exp \left[-\frac{1}{2} \phi^{\dagger} (h + h^{\dagger}) \phi + \phi^{\dagger} \kappa + \kappa^{\dagger} \phi \right]$$

$$= \exp \left[-\frac{1}{2} \ln \det(h + h^{\dagger}) + 2\kappa^{\dagger} (h + h^{\dagger})^{-1} \kappa \right],$$
(2.6)

where we use $\int D\phi = \prod_n \int D\phi_n$ with $D\phi_n = d\text{Re}\phi_n d\text{Im}\phi_n/\pi$ for complex fields and $D\phi_n = d\phi_n/\sqrt{\pi}$ for real fields. Canonical normalization corresponds to this expression being unity. More generally, the scalar product between a state functional $\Psi[\phi]$ specified by h, λ and κ and another one $\bar{\Psi}[\phi]$ specified by \bar{h} , $\bar{\lambda}$ and $\bar{\kappa}$ is given by the functional integral

$$\langle \bar{\Psi} | \Psi \rangle = \int D\phi \, \exp \left[-\frac{1}{2} \phi^{\dagger} (h + \bar{h}^{\dagger}) \phi + \frac{i}{2} \phi^{\dagger} (\lambda - \bar{\lambda}) + \frac{i}{2} (\lambda - \bar{\lambda})^{\dagger} \phi + \frac{1}{2} \phi^{\dagger} (\kappa + \bar{\kappa}) + \frac{1}{2} (\kappa + \bar{\kappa})^{\dagger} \phi \right]. \tag{2.7}$$

Using two sets of eigenstates of (2.3), whose eigenvalues we denote by ϕ_+ and ϕ_- , the pure-state density matrix can be written as

$$\rho_{\lambda,\kappa}[\phi_{+},\phi_{-}] = \langle \phi_{+}|\Psi\rangle\langle\Psi|\phi_{-}\rangle
= \exp\left[-\frac{1}{2}\phi_{+}^{\dagger}h\phi_{+} - \frac{1}{2}\phi_{-}^{\dagger}h^{\dagger}\phi_{-} + \frac{i}{2}(\phi_{+}^{\dagger} - \phi_{-}^{\dagger})\lambda + \frac{i}{2}\lambda^{\dagger}(\phi_{+} - \phi_{-}) + \frac{1}{2}(\phi_{+}^{\dagger} + \phi_{-}^{\dagger})\kappa + \frac{1}{2}\kappa^{\dagger}(\phi_{+} + \phi_{-})\right].$$
(2.8)

The condition for a pure state density matrix $\text{Tr}\{\rho_{\lambda,\kappa}^2\}/\text{Tr}\{\rho_{\lambda,\kappa}\}^2=1$ is satisfied as it should be. We will also work with the canonically conjugate momentum field π_m . In the Schrödinger representation employed, it is given by a functional derivative operator

$$\pi_m = -i\frac{\delta}{\delta\phi_m} \,. \tag{2.9}$$

The representation (2.9) implies the canonical commutation relations

$$[\phi_m, \pi_m] = i\delta_{mn}, \qquad [\phi_m, \phi_n] = [\pi_m, \pi_n] = 0,$$
 (2.10)

and correspondingly for the complex conjugate fields.

2.3 Gaussian density matrices

The Gaussian density matrix we discussed was for a pure state. In the following, we will make the transition to mixed states in terms of the density matrix, but restrict ourselves to situations where the density matrix remains of the Gaussian form². We can write such a mixed state density matrix in the form,

$$\rho[\phi_{+},\phi_{-}] = \int D\lambda D\kappa P[\lambda,\kappa] \rho_{\lambda,\kappa}[\phi_{+},\phi_{-}], \qquad (2.11)$$

²Deviations from Gaussianity can be treated in this formalism perturbatively but shall not be discussed any further here.

where $\rho_{\lambda,\kappa}[\phi_+,\phi_-]$ is the pure state density matrix in (2.8) (dependent on the fields λ and κ) and $P[\lambda,\kappa]$ is a quasi-probability distribution. When positive, $P[\lambda,\kappa]$ can be seen as the probability distribution for statistical noise in the parameter fields λ and κ . More generally, however, $P[\lambda,\kappa]$ need not be positive semi-definite. (The density operator ρ should of course be hermitian and positive semi-definite.) Note that eq. (2.11) is closely related (although not identical) to the Glauber-P representation of a density matrix [7, 8].

In the following we will take $P[\lambda, \kappa]$ to also be of the Gaussian form,

$$P[\lambda, \kappa] = \exp\left[-\left(\lambda^{\dagger} - j^{\dagger}, \kappa^{\dagger}\right) \Sigma^{-1} {\lambda - j \choose \kappa} + \text{const}\right], \qquad (2.12)$$

with a hermitian operator Σ that we take to be of the form³

$$\Sigma = \Sigma^{\dagger} = \begin{pmatrix} \Sigma_a & i\Sigma_b \\ -i\Sigma_b & \Sigma_a \end{pmatrix}, \quad \text{with} \quad \Sigma_a = \Sigma_a^{\dagger}, \ \Sigma_b = \Sigma_b^{\dagger}.$$
 (2.13)

For this to be a properly normalizable probability distribution, the eigenvalues of Σ should be positive. One may also introduce the linearly transformed parameter fields,

$$\mu_m = \frac{i}{\sqrt{2}}(\lambda_m - j_m) + \frac{1}{\sqrt{2}}\kappa_m, \qquad \nu_m = -\frac{i}{\sqrt{2}}(\lambda_m - j_m) + \frac{1}{\sqrt{2}}\kappa_m,$$
 (2.14)

in terms of which the exponent in (2.12) becomes diagonal,

$$P[\mu, \nu] = \exp\left[-\mu^{\dagger} (\Sigma_a - \Sigma_b)^{-1} \mu - \nu^{\dagger} (\Sigma_a + \Sigma_b)^{-1} \nu + \text{const}\right]. \tag{2.15}$$

Substituting (2.12) in (2.11), one obtains straightforwardly that the mixed state density matrix $\rho[\phi_+,\phi_-]$ is also Gaussian. In the limit where $\Sigma\to 0$, the functional $P[\lambda]$ approaches a delta distribution functional and one recovers the pure state we started with. Performing the functional integral over λ and an overall shift of fields $\phi_+\to\phi_+-\bar{\phi}$, $\phi_-\to\phi_--\bar{\phi}$ gives

$$\rho[\phi_{+},\phi_{-}] = \exp\left[-\frac{1}{2}\left(\phi_{+}^{\dagger} - \bar{\phi}^{\dagger},\phi_{-}^{\dagger} - \bar{\phi}^{\dagger}\right)\begin{pmatrix}h & -\Sigma_{a} + \Sigma_{b}\\ -\Sigma_{a} - \Sigma_{b} & h^{\dagger}\end{pmatrix}\begin{pmatrix}\phi_{+} - \bar{\phi}\\ \phi_{-} - \bar{\phi}\end{pmatrix}\right) + \frac{i}{2}(\phi_{+}^{\dagger} - \phi_{-}^{\dagger})j + \frac{i}{2}j^{\dagger}(\phi_{+} - \phi_{-})\right].$$
(2.16)

We have introduced here the field $\bar{\phi}$ which corresponds to the field expectation value below.

Interestingly, this is the most general Gaussian density matrix that satisfies the hermiticity property

$$\rho[\phi_+, \phi_-] = \rho[\phi_-, \phi_+]^*. \tag{2.17}$$

As a consequence, any Gaussian density matrix can be written in the form (2.11) for suitable Gaussian $P[\lambda, \kappa]$.

The trace of (2.16) is given by

$$\operatorname{Tr}\{\rho\} = \int D\phi \ \rho[\phi, \phi] = \exp\left[-\frac{1}{2}\ln\det\left(h + h^{\dagger} - 2\Sigma_a\right)\right],\tag{2.18}$$

and in the following we will assume canonical normalization, $tr\{\rho\} = 1$, or divide by the appropriate power of the above expression.

 $^{^3}$ More general Gaussian forms for $P[\lambda, \kappa]$ are possible but will not be needed for our construction.

2.4 Projections and reduced density matrix

For the computation of the entanglement entropy and related quantities, we shall require reduced density matrices that result from performing partial traces over some of the degrees of freedom. Towards this end, one may introduce a projection operator $P = P^{\dagger} = P^2$ whereby

$$\tilde{\phi}_m = (\delta_{mn} - P_{mn})\phi_n^+ = (\delta_{mn} - P_{mn})\phi_n^- \tag{2.19}$$

are the fields we want to trace out, and

$$\hat{\phi}_m^{\pm} = P_{mn}\phi_n^{\pm} \tag{2.20}$$

are those we wish to retain. For example, P might be a projector in position space which equals unity in some interval and is zero in the complement region. The reduced density matrix is formally given by

$$\rho_R[\hat{\phi}_+, \hat{\phi}_-] = \int D\tilde{\phi} \, \rho[P\hat{\phi}^+ + (1-P)\tilde{\phi}, P\hat{\phi}^- + (1-P)\tilde{\phi}]. \tag{2.21}$$

(The projectors have been inserted here for clarity.) For the Gaussian density matrix (2.16), one can formally perform the functional integral over $\tilde{\phi}$ and obtain yet again a Gaussian form for the reduced density matrix,

$$\rho_{R}[\hat{\phi}_{+},\hat{\phi}_{-}] = \exp\left[-\frac{1}{2}\left((\hat{\phi}_{+}^{\dagger} - \bar{\phi}^{\dagger})P,(\hat{\phi}_{-}^{\dagger} - \bar{\phi}^{\dagger})P\right)\begin{pmatrix}h - d_{(++)} & -\Sigma_{a} + \Sigma_{b} - d_{(+-)} \\ -\Sigma_{a} - \Sigma_{b} - d_{(-+)} & h^{\dagger} - d_{(--)}\end{pmatrix}\begin{pmatrix}P(\phi_{+} - \bar{\phi}) \\ P(\phi_{-} - \bar{\phi})\end{pmatrix} + \frac{i}{2}(\phi_{+}^{\dagger} - \phi_{-}^{\dagger})Pj + \frac{i}{2}j^{\dagger}P(\phi_{+} - \phi_{-})\right].$$
(2.22)

We have used here the abbreviations

$$d_{(++)} = (h - \Sigma_a + \Sigma_b)(1 - P) \left[(1 - P)(h + h^{\dagger} - 2\Sigma_a)(1 - P) \right]^{-1} (1 - P)(h - \Sigma_a - \Sigma_b),$$

$$d_{(+-)} = (h - \Sigma_a + \Sigma_b)(1 - P) \left[(1 - P)(h + h^{\dagger} - 2\Sigma_a)(1 - P) \right]^{-1} (1 - P)(h^{\dagger} - \Sigma_a + \Sigma_b),$$

$$d_{(-+)} = (h^{\dagger} - \Sigma_a - \Sigma_b)(1 - P) \left[(1 - P)(h + h^{\dagger} - 2\Sigma_a)(1 - P) \right]^{-1} (1 - P)(h - \Sigma_a - \Sigma_b),$$

$$d_{(--)} = (h^{\dagger} - \Sigma_a - \Sigma_b)(1 - P) \left[(1 - P)(h + h^{\dagger} - 2\Sigma_a)(1 - P) \right]^{-1} (1 - P)(h^{\dagger} - \Sigma_a + \Sigma_b).$$
(2.23)

The operator inversions used here are to be done within the subspace that is integrated out. Note that the reduced density matrix (2.22) is of the same general structure as the original density matrix (2.16); in particular, it still satisfies the hermiticity property (2.17). However if one starts with the density matrix of a pure state where $\Sigma_a = \Sigma_b = 0$, the reduced density matrix (2.22) contains in general terms that mix ϕ_+ and ϕ_- (the terms $d_{(+-)}$ and $d_{(-+)}$ in (2.23)) and describes therefore a mixed state, as expected.

Because the reduced density matrix is again Gaussian, it is completely determined by the field expectation values and the two-field correlation functions. As we will discuss, these can be computed directly on the domain of interest without further reference to projection operators.

2.5 Correlation functions

A Gaussian density matrix can be completely characterized in terms of field expectation values and correlation functions of two fields. More specifically, for (2.11) one has for the field ϕ_m and the canonical conjugate momentum field $\pi_m = -i\delta/\delta\phi_m$,

$$\langle \phi_m \rangle = \frac{\int D\phi \, \phi_m \, \rho[\phi, \phi]}{\int D\phi \, \rho[\phi, \phi]} = \bar{\phi}_m, \qquad \langle \pi_m \rangle = \frac{\int D\phi \, (-i\delta\rho[\phi_+, \phi_-]/\delta\phi_{+m})_{\phi_+ = \phi_- = \phi}}{\int D\phi \, \rho[\phi, \phi]} = j_m^*. \quad (2.24)$$

For the connected correlation functions $\langle AB \rangle_c = \langle AB \rangle - \langle A \rangle \langle B \rangle$ one finds

$$\begin{split} \langle \phi_{m} \phi_{n}^{*} \rangle_{c} &= [(h + h^{\dagger} - 2\Sigma_{a})^{-1}]_{mn}, \\ \langle \pi_{m}^{*} \pi_{n} \rangle_{c} &= [h - (h - \Sigma_{a} + \Sigma_{b})(h + h^{\dagger} - 2\Sigma_{a})^{-1}(h - \Sigma_{a} - \Sigma_{b})]_{mn} \\ &= [h^{\dagger} - (h^{\dagger} - \Sigma_{a} - \Sigma_{b})(h + h^{\dagger} - 2\Sigma_{a})^{-1}(h^{\dagger} - \Sigma_{a} + \Sigma_{b})]_{mn} \\ &= [\Sigma_{a} - \Sigma_{b} + (h - \Sigma_{a} + \Sigma_{b})(h + h^{\dagger} - 2\Sigma_{a})^{-1}(h^{\dagger} - \Sigma_{a} + \Sigma_{b})]_{mn} \\ &= [\Sigma_{a} + \Sigma_{b} + (h^{\dagger} - \Sigma_{a} - \Sigma_{b})(h + h^{\dagger} - 2\Sigma_{a})^{-1}(h - \Sigma_{a} - \Sigma_{b})]_{mn}, \\ \langle \phi_{m} \pi_{n} \rangle_{c} &= i[(h + h^{\dagger} - 2\Sigma_{a})^{-1}(h - \Sigma_{a} - \Sigma_{b})]_{mn}, \\ \langle \pi_{n} \phi_{m} \rangle_{c} &= -i[(h + h^{\dagger} - 2\Sigma_{a})^{-1}(h^{\dagger} - \Sigma_{a} + \Sigma_{b})]_{mn}, \\ \langle \phi_{m}^{*} \pi_{n}^{*} \rangle_{c} &= i[(h - \Sigma_{a} + \Sigma_{b})(h + h^{\dagger} - 2\Sigma_{a})^{-1}]_{mn}, \\ \langle \pi_{n}^{*} \phi_{m}^{*} \rangle_{c} &= -i[(h^{\dagger} - \Sigma_{a} - \Sigma_{b})(h + h^{\dagger} - 2\Sigma_{a})^{-1}]_{mn}. \end{split}$$

These are compatible with the canonical commutation relations,

$$\langle \phi_m \pi_n - \pi_n \phi_m \rangle_c = i \delta_{mn},$$

$$\langle \phi_m^* \pi_n^* - \pi_n^* \phi_m^* \rangle_c = i \delta_{mn}.$$
(2.26)

Note that the matrices h, h^{\dagger} , Σ_a and Σ_b are fixed in terms of the connected correlation functions of ϕ , ϕ^* and the momenta π , π^* . For later convenience, we note the relations (using Einsteins summation convention)

$$a_{mn} \equiv [(h+h^{\dagger}-2\Sigma_{a})^{-1}\Sigma_{a}]_{mn} = \langle \phi_{m}\phi_{k}^{*}\rangle_{c}\langle \pi_{k}^{*}\pi_{n}\rangle_{c} - \frac{1}{4}\delta_{mn}$$

$$-\frac{1}{4}\langle \phi_{m}\phi_{k}^{*}\rangle_{c}\langle \phi_{k}^{*}\pi_{l}^{*} + \pi_{l}^{*}\phi_{k}^{*}\rangle_{c} [\langle \phi\phi^{*}\rangle_{c}]_{lr}^{-1}\langle \phi_{r}\pi_{n} + \pi_{n}\phi_{r}\rangle_{c},$$

$$b_{mn} \equiv [(h+h^{\dagger}-2\Sigma_{a})^{-1}\Sigma_{b}]_{mn} = \frac{i}{4}\langle \phi_{m}\pi_{n} + \pi_{n}\phi_{m}\rangle_{c} - \frac{i}{4}\langle \phi_{m}\phi_{k}^{*}\rangle_{c}\langle \phi_{k}^{*}\pi_{l}^{*} + \pi_{l}^{*}\phi_{k}^{*}\rangle_{c} [\langle \phi\phi^{*}\rangle_{c}]_{ln}^{-1}.$$

$$(2.27)$$

They follow with some algebra from (2.25).

2.6 Entropy and entanglement entropy

In this subsection we will determine the Rényi entropy for the general Gaussian density matrix (2.16) and extract from it the von Neumann entropy. The Rényi entropy is defined by (1.45). For the purposes of the calculation that follows, it is clear⁴ that one can drop $\bar{\phi}$ and j, as they do not enter tr{ ρ^N }. Using otherwise the general expression for ρ in (2.16) leads after a straight-forward exercise in Gaussian integration to [11]

$$\operatorname{Tr}\{\rho^N\} = \exp\left[-\frac{1}{2}\operatorname{Tr}\ln\det\left(\mathbb{M}_N\right)\right],$$
 (2.28)

which contains the N dimensional cyclic matrix (with operator valued entries)

$$\mathbb{M}_{N} = (1+2a)\mathbb{1}_{N} - (a+b)\mathbb{Z}_{N} - (a-b)\mathbb{Z}_{N}^{T}. \tag{2.29}$$

We have used here the abbreviations introduced in (2.27). We define further $\mathbb{1}_N$ to be the N-dimensional unit matrix and \mathbb{Z}_N is the N-dimensional cyclic matrix $(\mathbb{Z}_N)_{mn} = \delta_{(m+1)n}$. Here m, n are in the range $1, \ldots, N$ and the index m = N + 1 is to be identified with the index m = 1.

⁴This can be seen directly by writing out the expressions for $\operatorname{tr}\{\rho^N\}$ in the functional integral formalism or more formally by noting that $\bar{\phi}$ and j can be changed by unitary transformations.

One can write

$$\mathbf{M}_{N} = \mathbf{A}_{N}(a, b) \, \mathbf{A}_{N}^{T}(a^{T}, -b^{T}) \,, \tag{2.30}$$

with

$$A_N(a,b) = \left(\sqrt{\frac{1}{4} + a + b^2} + b + \frac{1}{2}\right) \mathbb{1}_N - \left(\sqrt{\frac{1}{4} + a + b^2} + b - \frac{1}{2}\right) \mathbb{Z}_N.$$
 (2.31)

The determinant of the matrix $A_N(a,b)$ is found to be

$$\det A_N(a,b) = \left(\sqrt{\frac{1}{4} + a + b^2} + b + \frac{1}{2}\right)^N - \left(\sqrt{\frac{1}{4} + a + b^2} + b - \frac{1}{2}\right)^N.$$
 (2.32)

Combining terms leads to a compact expression for the Rényi entropy,

$$S_N(\rho) = \frac{1}{2(N-1)} \left\{ \text{Tr} \ln \left(\left(\sqrt{\frac{1}{4} + a + b^2} + b + \frac{1}{2} \right)^N - \left(\sqrt{\frac{1}{4} + a + b^2} + b - \frac{1}{2} \right)^N \right) + \text{Tr} \ln \left(\left(\sqrt{\frac{1}{4} + a + b^2} - b + \frac{1}{2} \right)^N - \left(\sqrt{\frac{1}{4} + a + b^2} - b - \frac{1}{2} \right)^N \right) \right\}.$$

$$(2.33)$$

We have rederived here in general terms, and in the the functional integral representation, a result also known in the operator formalism [13], see also [12] and references therein.

From the result above, one can directly obtain an expression for the von Neumann entropy by taking the limit $N \to 1$,

$$S = \frac{1}{2} \operatorname{Tr} \left\{ \left(\sqrt{\frac{1}{4} + a + b^2} + b + \frac{1}{2} \right) \ln \left(\sqrt{\frac{1}{4} + a + b^2} + b + \frac{1}{2} \right) \right\}$$

$$- \frac{1}{2} \operatorname{Tr} \left\{ \left(\sqrt{\frac{1}{4} + a + b^2} + b - \frac{1}{2} \right) \ln \left(\sqrt{\frac{1}{4} + a + b^2} + b - \frac{1}{2} \right) \right\}$$

$$+ \frac{1}{2} \operatorname{Tr} \left\{ \left(\sqrt{\frac{1}{4} + a + b^2} - b + \frac{1}{2} \right) \ln \left(\sqrt{\frac{1}{4} + a + b^2} - b + \frac{1}{2} \right) \right\}$$

$$- \frac{1}{2} \operatorname{Tr} \left\{ \left(\sqrt{\frac{1}{4} + a + b^2} - b - \frac{1}{2} \right) \ln \left(\sqrt{\frac{1}{4} + a + b^2} - b - \frac{1}{2} \right) \right\}.$$

$$(2.34)$$

Note that this is positive semi-definite because a - b and a + b are positive semi-definite. Note also, that a and b can be expressed in terms of correlation functions of fields and canonical momenta using (2.27). The above expression simplifies for b = 0 to

$$S = \text{Tr}\left\{ \left(\sqrt{\frac{1}{4} + a} + \frac{1}{2} \right) \ln \left(\sqrt{\frac{1}{4} + a} + \frac{1}{2} \right) - \left(\sqrt{\frac{1}{4} + a} - \frac{1}{2} \right) \ln \left(\sqrt{\frac{1}{4} + a} - \frac{1}{2} \right) \right\}, \tag{2.35}$$

and it vanishes as expected for b = a = 0.

As a first example and check of this formalism, consider a free real massive scalar field in n-dimensional infinite Minkowski space. The correlation functions in this case can be written as

$$\Delta_{\phi\phi}^{S}(\vec{x}-\vec{y}) = \langle \phi(t,\vec{x})\phi(t,\vec{y})\rangle = \int_{\vec{p}} \frac{e^{i\vec{p}(\vec{x}-\vec{y})}}{\sqrt{\vec{p}^{2}+M^{2}}} \left[\frac{1}{2} + n(\vec{p})\right],$$

$$\Delta_{\pi\pi}^{S}(\vec{x}-\vec{y}) = \langle \pi(t,\vec{x})\pi(t,\vec{y})\rangle = \int_{\vec{p}} e^{i\vec{p}(\vec{x}-\vec{y})} \sqrt{\vec{p}^{2}+M^{2}} \left[\frac{1}{2} + n(\vec{p})\right],$$
(2.36)

where $n(\vec{p})$ are occupation numbers. The symmetric mixed correlation function vanishes: $\langle \phi \pi + \pi \phi \rangle / 2 = 0$ and therefore b = 0. Here one can evaluate the (full) entropy easily, because $a = (h + h^{\dagger})^{-1}\Sigma_a$ as given in (2.27) is diagonal in momentum space. One finds

$$S = \int_{\vec{p}} \{ (n(\vec{p}) + 1) \ln (n(\vec{p}) + 1) - n(\vec{p}) \ln (n(\vec{p})) \} , \qquad (2.37)$$

which is the standard result for free bosonic fields. As expected, the entropy vanishes for $n(\vec{p}) \to 0$.

2.7 Symplectic transformations, Williamson's theorem and entanglement entropy

The above expressions can be further simplified with the help of canonical transformations. One considers unitary changes of the field basis,

$$\phi_m \to U_{mn}\phi_n , \qquad \phi_m^* \to \phi_n^*(U^\dagger)_{nm} ,$$

$$\pi_m^* \to U_{mn}\pi_n^* , \qquad \pi_m \to \pi_n(U^\dagger)_{nm} .$$
(2.38)

They can be used to diagonalize hermitian operators such as $h + h^{\dagger}$ as is the case in going from position to momentum space. These transformations have unitary representations as transformations of the Schrödinger functionals. This is clear as the scalar product (2.7) remains unchanged by unitary transformations of the field basis due to $D\phi = D(U\phi)$.

In addition to this, there is a larger class of transformations, which transform fields and momenta into each other. Consider the combined field

$$\chi = \begin{pmatrix} \phi \\ \pi^* \end{pmatrix}, \qquad \chi^* = \begin{pmatrix} \phi^* \\ \pi \end{pmatrix}.$$
(2.39)

Their canonical commutation relation defines a symplectic metric,

$$\left[\chi_m, \chi_n^*\right] = \Omega_{mn} \,, \tag{2.40}$$

where, symbolically,

$$\Omega = \Omega^{\dagger} = \begin{pmatrix} 0 & i\mathbb{1} \\ -i\mathbb{1} & 0 \end{pmatrix}. \tag{2.41}$$

The transformations

$$\chi_m \to S_{mn} \chi_n, \qquad \chi_m^* \to \chi_n^* (S^\dagger)_{nm}, \qquad (2.42)$$

such that

$$S\Omega S^{\dagger} = \Omega, \tag{2.43}$$

are compatible with the canonical commutation relations. This defines a symplectic transformation. Written in terms of the Lie algebra, $S = \exp[i\theta^A J^A]$, the condition (2.43) becomes

$$\Omega J^A = (J^A)^{\dagger} \Omega \,. \tag{2.44}$$

Indeed one can confirm that this relation defines a Lie algebra.

Recall that ϕ and π contain also the corresponding complex conjugate fields so that there are relations

$$\chi_m^* = R_{mn} \chi_n, \qquad \chi_n = R_{nm}^{-1} \chi_m^* = \chi_m^* (R^{\dagger})_{mn}.$$
(2.45)

One may assume without loss of generality that there is a field basis where all fields are real such that there $R_{mn} = \delta_{mn}$. Of course, the matrix R changes under the unitary, block diagonal transformations (2.38). More specifically, one has

$$R \to U^* R(U^{\dagger})$$
. (2.46)

The matrix R transforms also by the symplectic transformations (2.42),

$$R \to S^* R(S^{-1})$$
. (2.47)

Notice that in the field basis where ϕ_m is real, there is no change in R for real symplectic transformations. Hence $S_{mp}^* = S_{mp}$, as expected. In a field basis that differs from this by a unitary transformation, the symplectic transformation has different form (and is not necessarily real). Specifically,

the symplectic transformation matrix in (2.42) and the generator J^A transform under the unitary block diagonal transformations (2.38) as

$$S \to USU^{\dagger}, \qquad J^A \to UJ^AU^{\dagger}.$$
 (2.48)

We need to show that the symplectic transformations (2.42) have unitary representations as transformations of the states of the field theory. This is best done in the field basis where ϕ_m are real fields and R = 1. The symplectic transformations are then real and one has

$$J^{A} = -(J^{A})^* = \Omega(J^{A})^{\dagger} \Omega = -\Omega(J^{A})^T \Omega. \tag{2.49}$$

There is now a representation of the Lie algebra specified by (2.44) in terms of the operators ([14], see also [15])

$$X^{A} = \frac{1}{2} \chi_{m}^{*} \Omega_{mn} (J^{A})_{nk} \chi_{k} , \qquad (2.50)$$

acting on a Schrödinger functional. Indeed, one can confirm that they have the same commutation relations as the generators J^A . Moreover, one has $(X^A)^{\dagger} = X^A$ in the sense of the bilinear form (2.7) so that the symplectic transformations indeed have unitary representations. This is an important result because it allows one to use the symplectic transformations to simplify calculations, for example of the entropy. Because symplectic transformations have unitary representations, they do not change the entropy by construction.

Finally, we note that (2.50) is invariant under the block diagonal unitary transformations (2.38) and can therefore be used in any field basis. It is also clear that the corresponding unitary transformation maps Gaussian states to Gaussian states.

In particular, the hermitian and positive covariance matrix corresponding to the symmetrized correlation function

$$\Delta_{mn} = \frac{1}{2} \langle \chi_m \chi_n^* + \chi_n^* \chi_m \rangle_c = \begin{pmatrix} \langle \phi_m \phi_n^* \rangle_c & \frac{1}{2} \langle \phi_m \pi_n + \pi_n \phi_m \rangle_c \\ \frac{1}{2} \langle \pi_m^* \phi_n^* + \phi_n^* \pi_m^* \rangle_c & \langle \pi_m^* \pi_n \rangle_c , \end{pmatrix},$$
(2.51)

which is a key ingredient in our discussion of Gaussian states, transforms under symplectic transformations as

$$\Delta \to S\Delta S^{\dagger}$$
. (2.52)

This is not a similarity transformation because $S^{\dagger} \neq S^{-1}$. In other words, the eigenvalues of Δ are not invariant under symplectic transformations. Williamson's theorem states (see [16] for a discussion) however that there must exist a symplectic transformation that brings Δ to diagonal form.

$$\Delta = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_1, \lambda_2, \dots), \tag{2.53}$$

with real and positive $\lambda_j > 0$. These latter are the *symplectic eigenvalues* of the symmetrized covariance matrix.

This is realized by considering the combination $\Delta\Omega$. One can show that it transforms as

$$\Delta\Omega \to S\Delta S^{\dagger}\Omega = S\Delta\Omega S^{-1} \,, \tag{2.54}$$

which indeed satisfies the properties of a similarity transformation. The eigenvalues of this combination, $\pm \lambda_j$, are directly related to the symplectic eigenvalues. It is therefore convenient to determine the eigenvalues of $\Delta\Omega$ and to thereby relate observables such as the entanglement entropy to the Williamson form.

We first note that the Williamson form expression (2.53) of the symmetric correlation matrix (2.51) results in a very simple form for the quantities in (2.27):

$$a_{ij} = \left(\lambda_j^2 - \frac{1}{4}\right) \delta_{ij}, \qquad b_{ij} = 0.$$
 (2.55)

Since the Heisenberg uncertainty relation tells us that a_{ij} has to be positive-definite, this indicates that $\lambda_i \geq 1/2$.

The symplectic transformations we have discussed and the resulting use of Williamson's theorem leads to a very convenient form for entropies. The entropy in (2.35) can be directly expressed in terms of the symplectic eigenvalues as

$$S = \sum_{j} \left\{ \left(\lambda_j + \frac{1}{2} \right) \ln \left(\lambda_j + \frac{1}{2} \right) - \left(\lambda_j - \frac{1}{2} \right) \ln \left(\lambda_j - \frac{1}{2} \right) \right\}. \tag{2.56}$$

Moreover, the symplectic eigenvalues λ_m follow as pairs of conventional eigenvalues $\pm \lambda_j$ of the combination $\Delta\Omega$. Following Sorkin ([17], see also [18]), a further simplification can be obtained by considering the matrix

$$D = \Delta\Omega + \frac{1}{2}\mathbb{1}\,,\tag{2.57}$$

which has the eigenvalues $\omega_j^+ = 1/2 + \lambda_j$ and $\omega_j^- = 1/2 - \lambda_j$. As noted, the uncertainty relation gives us $\lambda_j \geq 1/2$; therefore, $\omega_j^+ \geq 1$ and $\omega_j^- \leq 0$. One can then write (2.56) simply as

$$S = \sum_{j} \left\{ \omega_{j}^{+} \ln(\omega_{j}^{+}) + \omega_{j}^{-} \ln(-\omega_{j}^{-}) \right\} , \qquad (2.58)$$

where the sum is over pairs of eigenvalues. More simply,

$$S = \sum_{m} \omega_m \ln(|\omega_m|) = \frac{1}{2} \operatorname{Tr} \left\{ D \ln(D^2) \right\}.$$
 (2.59)

In the last expression, the sum is now over all the eigenvalues of D. Each negative eigenvalue $\omega_m < 0$ is paired with a positive one $1 - \omega_m$. A pure state without entropy has $\omega_m \in \{0, 1\}$. Finally, we note that the matrix D in symbolic form can be expressed as

$$D_{mn} = \begin{pmatrix} \frac{1}{2}\mathbb{1} - \frac{i}{2}\langle\phi_m\pi_n + \pi_n\phi_m\rangle_c & i\langle\phi_m\phi_n^*\rangle_c \\ -i\langle\pi_m^*\pi_n\rangle_c & \frac{1}{2}\mathbb{1} + \frac{i}{2}\langle\pi_m^*\phi_n^* + \phi_n^*\pi_m^*\rangle_c \end{pmatrix} = \begin{pmatrix} -i\langle\phi_m\pi_n\rangle_c & i\langle\phi_m\phi_n^*\rangle_c \\ -i\langle\pi_m^*\pi_n\rangle_c & i\langle\pi_m^*\phi_n^*\rangle_c \end{pmatrix}. (2.60)$$

Hence, the entropy associated with a Gaussian density matrix is fully determined from the set of connected correlation functions of (2.60) evaluated in the domain of interest. It is understood that the operator trace in (2.59) is also restricted to this domain.

Thus far, we have concentrated on the Rényi and von Neumann entropies of a single Gaussian density matrix. It is also possible to determine relative entropies between two Gaussian density matrices ρ and σ in a similar way. Let us remark here that Williamson's theorem is not as useful for the determination of the relative entropy of two Gaussian density matrices as it is for the determination of the entropy of a single one. This is because it is not guaranteed that there is a basis in which the covariance matrices $\Delta^{(\rho)}$ and $\Delta^{(\sigma)}$ (defined in (2.51)) simultaneously assume their Williamson diagonal form. However, this should be the case when the matrices $\Delta^{(\rho)}\Omega$ and $\Delta^{(\sigma)}\Omega$ (which transform under symplectic transformations as similarity transforms, see (2.54)) commute, i.e. $[\Delta^{(\rho)}\Omega, \Delta^{(\sigma)}\Omega] = 0$. One can then write the relative entropy as

$$S(\rho|\sigma) = \sum_{m} \omega_{m}^{(\rho)} \left(\ln|\omega_{m}^{(\sigma)}| - \ln|\omega_{m}^{(\rho)}| \right), \tag{2.61}$$

where the sum goes over all pairs of simultaneous eigenvalues $(\omega_m^{(\rho)}, \omega_m^{(\sigma)})$ of $D^{(\rho)} = \Delta^{(\rho)}\Omega + \frac{1}{2}\mathbb{1}$ and $D^{(\sigma)} = \Delta^{(\sigma)}\Omega + \frac{1}{2}\mathbb{1}$.

2.8 Gaussian reduced density matrices

Now that we have laid out the general formalism, one can apply it to determine the entropy or entanglement entropy for various situations. Equations (2.34) with (2.27) or (2.59) with (2.60) make clear, that the knowledge of the connected correlation functions of fields and canonically conjugate momenta on some hypersurface Σ is sufficient to determine the entropy. In this regard, the only difference between the determination of an entropy and an entanglement entropy is the space on which the traces in (2.34) or (2.59) are taken. To calculate the full entropy, the trace is to be taken on the entire space (or hypersurface), while to calculate the entanglement entropy of a subregion, the trace must be restricted to that subregion. In the latter case, only correlation functions in the subregion enter, of course.

It is important to realize that the correlation functions for a subregion are for a given quantum state in fact the same correlation functions as for the entire space – they are only restricted in the sense that they are evaluated only for points in the region of interest. A useful recipe is therefore to first determine the needed correlation functions for the entire space, then evaluate them on the region of interest and afterwards perform the diagonalizations and traces needed to evaluate (2.34) or (2.59). Below we will illustrate the procedure for an interval in d = 1 + 1 dimensional Minkowski space.

2.9 Finite interval in Minkowski space

We will consider an interval (-L/2, L/2) in Minkowski space with one spatial dimension. A free scalar field ϕ will be governed by a Gaussian reduced density matrix on this interval. Moreover, the corresponding matrix entries, namely the functions h, h^{\dagger} , Σ_a and Σ_b introduced in section 2, will be such that the correlation functions have the same form as in infinite space; they are just restricted to the interval. The technical difficulties arise now from the fact that products of these functions involve integrals over the interval (-L/2, L/2), only. For example, the quantity $a = (h + h^{\dagger} - 2\Sigma_a)^{-1}\Sigma_a$ defined in (2.27) becomes

$$a(x,y) = \int_{-L/2}^{L/2} dz \, \Delta_{\phi\phi}^{S}(x-z) \Delta_{\pi\pi}^{S}(z-y) - \frac{1}{4}\delta(x-y)$$

$$= \int_{p,q} \left\{ \frac{\sqrt{q^2 + M^2}}{4\sqrt{p^2 + M^2}} \frac{\sin\left(\frac{1}{2}(p-q)L\right)}{\frac{1}{2}(p-q)} - \frac{2\pi}{4}\delta(p-q) \right\} e^{ipx - iqy}.$$
(2.62)

We have used here

$$\Delta_{\phi\phi}^{S}(x-y) = \frac{1}{2} \langle \phi(x)\phi(y) + \phi(y)\phi(x) \rangle,$$

$$\Delta_{\pi\pi}^{S}(x-y) = \frac{1}{2} \langle \pi(x)\pi(y) + \pi(y)\pi(x) \rangle,$$
(2.63)

and the fact that the symmetrized mixed correlation function vanishes.

Note that this is a nondiagonal matrix in momentum space for finite L. Only in the limit $L \to \infty$ does one obtain $\sin(\frac{1}{2}(p-q)L)/(\frac{1}{2}(p-q)) \to (2\pi)\delta(p-q)$ and a becomes diagonal in momentum space (and zero). The challenge is now to find the eigenvalues of the matrix a(x,y) on the interval (-L/2,L/2).

To solve the eigenvalue problem, we will use a discrete basis involving Fourier expansion on the interval (-L/2, L/2). In doing so, we will not assume periodic boundary conditions. We first divide the relevant function (or field) into a symmetric and an anti-symmetric part,

$$\varphi(x) = \varphi^{(s)}(x) + \varphi^{(a)}(x), \qquad \varphi^{(s)}(x) = \frac{\varphi(x) + \varphi(-x)}{2}, \qquad \varphi^{(a)}(x) = \frac{\varphi(x) - \varphi(-x)}{2}.$$
 (2.64)

The symmetric part can be expanded into a Fourier series

$$\varphi^{(s)}(x) = \frac{1}{L} \sum_{\substack{n = -\infty \\ n \text{ even}}}^{\infty} \varphi_n \ e^{in\pi x/L}, \qquad \varphi_n = \int_{-L/2}^{L/2} dx \ \varphi^{(s)}(x) \ e^{-in\pi x/L} \quad (n \text{ even}).$$
 (2.65)

In a similar fashion, one can expand the anti-symmetric part

$$\varphi^{(a)}(x) = \frac{1}{L} \sum_{\substack{n = -\infty \\ n \text{ odd}}}^{\infty} \varphi_n \ e^{in\pi x/L}, \qquad \varphi_n = \int_{-L/2}^{L/2} dx \ \varphi^{(a)}(x) \ e^{-in\pi x/L} \quad (n \text{ odd}).$$
 (2.66)

We can summarize this as

$$\varphi(x) = \frac{1}{L} \sum_{n = -\infty}^{\infty} \varphi_n \ e^{in\pi x/L}, \qquad \varphi_n = \int_{-L/2}^{L/2} dx \ \varphi(x) \ \frac{1}{2} \left[e^{-in\pi x/L} + (-1)^n e^{in\pi x/L} \right] \ . \tag{2.67}$$

For $\varphi(x) \in \mathbb{R}$, one has $\varphi_n = \varphi_{-n}^*$. Note that this type of Fourier expansion does not assume periodic boundary conditions for $\varphi(x)$.

The so constructed discrete Fourier basis can be used to find a discrete (but still infinite) representation of correlation functions. If one truncates the discrete spectrum in the UV, one obtains a finite representation that can be used for a numerical diagonalization and determination of the entanglement entropy. Details can be found in ref. [5]. An alternative numerical treatment works entirely on a lattice discretization of the quantum field theory, see [12] for details.

The result for the entanglement entropy of a finite interval is in fact UV divergent. For a single free, massless, real scalar field in d = 1 + 1 dimensions one finds for the entanglement entropy

$$S_L = \frac{1}{3}\ln(L\Lambda) + \text{const}, \qquad (2.68)$$

where Λ is a UV momentum cutoff function and the additive constant is not universal in the sense that it depends on how precisely the UV regulator is implemented. What is universal is the so-called entropy c-function that is given here by

$$c(L) = L\frac{\partial}{\partial L}S_L = \frac{1}{3}.$$
(2.69)

More general, for massive theories c(L) depends actually on the interval length, or more specifically on the dimensionless product ML. Moreover, for theories with more than a single field, c is proportional to the "number of degrees of freedom" which means here number of independent scalar fields but counts more generally also Dirac fields etc.

3 Modular or entanglement hamiltonians

In this section we will be concerned directly with the form of the density matrix ρ for global as well as local descriptions of quantum fields.

3.1 Density matrices in quantum field theory

In section 1 we have discussed extensively Gaussian density matrices. This is an important class of states, in particular for free field theories or perturbative extensions. Here we will be interested in more general descriptions of density matrices for quantum fields.

What is a typical form of the density matrix? Beyond the Gaussian case, a particularly important class of density matrices concerns thermal states. This can be formulated also non-perturbatively. Vacuum or ground states are part of this class in the limit of vanishing temperature $T \to 0$.

A thermal equilibrium is defined on some space-like hypersurface Σ of space-time and in general coordinates as

$$\rho = \frac{1}{Z} \exp\left[-\int d\Sigma_{\mu} \beta_{\nu}(x) T^{\mu\nu}(x)\right]. \tag{3.1}$$

Here Z is a normalization factor such that $\operatorname{tr}\{\rho\}=1$, the hypersurface volume element is $d\Sigma_{\mu}=\sqrt{g}n_{\mu}(x)d^{3}x=\sqrt{g}\epsilon_{\mu\alpha\beta\gamma}dx^{\alpha}dx^{\beta}dx^{\gamma}/3!$ with normal vector n_{μ} and $\sqrt{g}=\sqrt{-\det g_{\mu\nu}}$. The vector $\beta_{\nu}(x)$ is defined by

$$\beta^{\nu}(x) = \frac{u^{\nu}(x)}{T(x)},\tag{3.2}$$

where $u^{\nu}(x)$ is the fluid velocity and T(x) the temperature and $T^{\mu\nu}(x)$ is the energy-momentum tensor of the quantum fields. One can show that the state (3.1) describes a global equilibrium state if $\beta^{\nu}(x)$ is a Killing vector field, so that it satisfies

$$\nabla_{\mu}\beta_{\nu}(x) + \nabla_{\nu}\beta_{\mu}(x) = 0. \tag{3.3}$$

Alternatively, in a conformal field theory it is sufficient if $\beta^{\nu}(x)$ is a conformal Killing vector field (this is a weaker condition) and satisfies with some function $\kappa(x)$ the relation

$$\nabla_{\mu}\beta_{\nu}(x) + \nabla_{\nu}\beta_{\mu}(x) - \kappa(x)g_{\mu\nu}(x) = 0. \tag{3.4}$$

One can also extend the state (3.1) to (local) thermal equilibrium with a chemical potential $\mu(x)$ as well as more general states which also have coherent fields, order parameters and so on.

3.2 Imaginary time and Matsubara formalism

For global thermal equilibrium states there is a very useful geometric representation. In the fluid rest frame and in cartesian coordinates one has

$$\rho = \frac{1}{Z}e^{-\frac{1}{T}H},\tag{3.5}$$

which resembles closely the time evolution operator for a time interval Δt ,

$$U(\Delta t) = e^{-i\Delta tH}. (3.6)$$

Expectation values or correlation functions of the form $\operatorname{tr}\{\rho\mathcal{O}\}\$ can be calculated by a functional integral on a geometry with periodicity in imaginary time such that bosonic fields satisfy $\varphi(t, \mathbf{x}) = \varphi(t - i\frac{1}{T}, \mathbf{x})$. This leads to the Matsubara formalism for quantum fields at non-vanishing temperature.

In other words, quantum fields at finite temperature are described by a geometry with periodicity in imaginary time direction. In a general coordinate system, the periodic structure is

$$\varphi(x^{\mu}) = \pm \varphi(x^{\mu} - i\beta^{\mu}(x)), \tag{3.7}$$

where the minus sign holds for fermionic fields.

The von Neumann entropy of a thermal state (3.5) follows with $Z = e^{-\frac{1}{T}F}$, where F = E - TS is the free energy with differential dF = -SdT - pdV. Indeed, it is given by

$$S(\rho) = -\operatorname{tr}\{\rho \ln \rho\} = \frac{1}{T}(\langle H \rangle - F) = S. \tag{3.8}$$

3.3 Relative entropy characterization of locally thermal states

It is interesting to consider the quantum relative entropy $S(\rho||\sigma)$ for the special case where $\sigma = \frac{1}{Z}e^{-\beta H}$ is a thermal density matrix (3.5). The relative entropy becomes

$$S(\rho||\sigma) = \text{Tr}\{\rho \ln \rho\} + \beta \left(\langle H \rangle_{\rho} - F_{\sigma}\right)$$

= $-S_{\rho} + S_{\sigma} + \beta \left(\langle H \rangle_{\rho} - \langle H \rangle_{\sigma}\right),$ (3.9)

where $\langle \cdot \rangle_{\rho}$ and $\langle \cdot \rangle_{\sigma}$ denote expectation values with respect to the density matrices ρ and σ , respectively, while S_{ρ} and S_{σ} denote the corresponding von Neumann entropies. Possible UV divergent contributions to the entanglement entropy are independent of the state and cancel between the first and second term in the second line of (3.9). (This is actually a general statement independent of the specific choice for σ made here.) Moreover, also possibly UV divergent contributions to the expectation values of energy, e. g. from the zero-point fluctuations of various modes cancel on the right hand side of (3.9). Note that for equal energy, $\langle H \rangle_{\rho} = \langle H \rangle_{\sigma}$, the relative entropy (3.9) equals the difference of entropies.

We may also consider a density matrix ρ of the local thermal equilibrium form (3.1). If ρ_1 is obtained from ρ by an excitation generated by a unitary (entropy preserving) operation such that $S(\rho) = S(\rho_1)$, we may write the relative entropy

$$S(\rho_1||\rho) = \int_{\Sigma} d\Sigma_{\mu} \beta_{\nu} \left[\langle T^{\mu\nu} \rangle_{\rho_1} - \langle T^{\mu\nu} \rangle_{\rho} \right]. \tag{3.10}$$

In particular, if β_{ν} is constant in the region where $[\langle T^{\mu\nu}\rangle_{\rho_1} - \langle T^{\mu\nu}\rangle_{\rho}]$ is non-vanishing, we can write

$$S(\rho_1||\rho) = \beta_{\nu} \Delta \mathscr{P}^{\nu}, \tag{3.11}$$

where

$$\Delta \mathscr{P}^{\nu} = \int_{\Sigma} d\Sigma_{\mu} \left[\langle T^{\mu\nu} \rangle_{\rho_{1}} - \langle T^{\mu\nu} \rangle_{\rho} \right]$$
 (3.12)

is the integrated energy-momentum of the excitation. Note that (3.10) is reminiscent of the definition of temperature in the grand canonical ensemble

$$dS = \frac{1}{T}dE. (3.13)$$

These considerations can partly be extended away from the case where σ is thermal in terms of the so-called *modular or entanglement Hamiltonian*, defined here for the density matrix σ as the operator

$$K = -\ln \sigma, \qquad \sigma = e^{-K}. \tag{3.14}$$

The relative entropy $S(\rho||\sigma)$ becomes then

$$S(\rho||\sigma) = -S_{\rho} + \langle K \rangle_{\rho} = -S_{\rho} + S_{\sigma} + \langle K \rangle_{\rho} - \langle K \rangle_{\sigma} \ge 0. \tag{3.15}$$

The modular or entanglement Hamiltonian can be defined for any density matrix. (For Gaussian density matrices it is quadratic in the fields.) However, it is usually not of a particularly simple form, except if the density matrix is thermal. Of course, as the name indicates, one is typically interested in the case where the density matrix is in fact a reduced density matrix, obtained by tracing out certain regions of space, for example. In some situations, the entanglement Hamiltonian defined in this way can actually be determined as we will discuss below.

3.4 Rindler wedge and its horizon

Consider a constant time surface in Minkowski space at t=0 and divide it into two parts: region A corresponds to x>0 and region B to $x\leq 0$. (For simplicity we consider a field theory in d=1+1 dimensions but the generalization to higher dimensions is straight forward.) We will consider the standard Minkowski vacuum state of a quantum field theory and want to characterize the reduced density matrix

$$\rho_A = \operatorname{tr}_B\{\rho\}. \tag{3.16}$$

We will use geometric methods to determine the reduced density matrix ρ_A and the corresponding entanglement Hamiltonian.

Consider the Rindler coordinate system (do not confuse ρ and σ with density matrices here)

$$t = \rho \sinh(\sigma), \qquad x = \rho \cosh(\sigma).$$
 (3.17)

Here, $\rho > 0$ corresponds to a spatial coordinate and σ is a new time coordinate. In particular t=0 corresponds to $\sigma=0$ and $\rho=x$ there. The coordinate system (3.17) covers only the part x>|t| of Minkowski space, called the *Rindler wedge*. Lines of constant ρ correspond to trajectories of observers with constant acceleration $a=1/\rho$. Note that this class of observers experiences a horizon at $\rho=0$ corresponding to the light cone x=|t|. Signals that are sent across this line are never coming back into the Rindler wedge.

The Minkowski space metric becomes in Rindler coordinates

$$ds^{2} = -dt^{2} + dx^{2} = -\rho^{2}d\sigma^{2} + d\rho^{2}.$$
(3.18)

3.5 Unruh effect

Interestingly, translations in the new time coordinate $\sigma \to \sigma + \Delta \sigma$ correspond to a symmetry of Minkowski space, namely Lorentz boosts in x-direction around the origin t = x = 0. The operator

$$U = e^{-i\Delta\sigma K} \tag{3.19}$$

corresponds to a Lorentz boost from the point of view of the cartesian coordinate system in Minkowski space and to a time translation from the point of view of Rindler coordinates. In other words, K plays the role of a Hamiltonian for the Rindler observers.

One may ask what happens if one analytically continues the time coordinate σ to imaginary values $\sigma = -i\eta$. Equation (3.17) becomes

$$t = -i\rho\sin(\eta), \qquad x = \rho\cos(\eta).$$
 (3.20)

This is just a parametrization of Euclidean space corresponding to the analytic continuation to imaginary times from Minkowski space. In particular, what corresponds to boosts in Minkowski space is now just a rotation in Euclidean space. In particular, the Euclidean coordinate η is periodic in the sense that η and $\eta + 2\pi$ correspond to the same point.

In other words, Rindler space is in fact periodic in imaginary Rindler time direction $\sigma = -i\eta$. This is precisely the characteristic of a thermal state! The fluid velocity points in the direction of time translations. To find the temperature, note that $\rho d\eta$ is periodic after rotation $\frac{1}{T} = 2\pi\rho$, corresponding to the Unruh temperature of Rindler space

$$T = \frac{1}{2\pi\rho}. (3.21)$$

Restoring units and taking into account that the acceleration is $a=1/\rho$ leads to the acceleration dependent *Unruh temperature*

$$T = \frac{\hbar a}{2\pi k_B c}. ag{3.22}$$

Note that we made no specific assumption on the field theory except for a Lorentz-invariant ground state. One therefore expects the Unruh effect to be rather universal. In particular, it holds for both massless and massive theories, as well as both non-interacting and interacting theories. One may also check that the "inverse temperature vector" $\beta^{\mu} = (2\pi\rho, 0)$ in Rindler coordinates or

$$\beta^{\mu} = \frac{1}{T} u^{\mu} = 2\pi \rho \begin{pmatrix} \cosh(\sigma) \\ \sinh(\sigma) \end{pmatrix} = 2\pi \begin{pmatrix} x \\ t \end{pmatrix}, \tag{3.23}$$

in Minkowski coordinates, is in fact a Killing vector, i. e. it satisfies the condition in equation (3.3).

We can now come back to the original problem to determine the reduced density matrix ρ_A on the half space x > 0 at t = 0. It is given by

$$\rho_A = \frac{1}{Z} \exp\left[-\int d\Sigma_\mu \beta_\nu T^{\mu\nu}\right] = \frac{1}{Z} \exp\left[-\int_0^\infty dx \, 2\pi x \, \mathcal{H}(x)\right],\tag{3.24}$$

with Hamiltonian density of the quantum field theory $T^{00} = \mathcal{H}$. Indeed, this corresponds to a thermal density matrix with space-dependent temperature $T = 1/(2\pi x)$. In particular, the temperature diverges when one approaches the boundary $x \to 0_+$.

Note that the interpretation of the thermal character of the state described by ρ_A is rather subtle. The state is vacuum-like and in particular has the same expectation values and correlation functions as the Minkowski space vacuum (when the latter is restricted to the Rindler wedge and with the correct identification of coordinate points of course). In other words, one simply has to probe the Minkowski space vacuum on the right accelerated trajectory to find thermal correlation functions!

3.6 Hawking radiation, temperature and entropy of black holes

A Schwarzschild black hole with mass M has the metric

$$ds^{2} = -\left(1 - \frac{2G_{N}M}{r}\right)dt^{2} + \left(1 - \frac{2G_{N}M}{r}\right)^{-1}dr^{2} + r^{2}d\Omega^{2}.$$
 (3.25)

Note that at the horizon, $r = 2G_{\rm N}M$, the signs of the coefficients in front of dt^2 and dr^2 change and time t and radius r effectively change their role for $r < 2G_{\rm N}M$. We consider now the region just outside the horizon

$$r = 2G_{\rm N}M + \frac{\rho^2}{8G_{\rm N}M},\tag{3.26}$$

and find for the metric to lowest order in ρ

$$ds^{2} = \frac{\rho^{2}}{16(G_{N}M)^{2}}dt^{2} + d\rho^{2} + (2G_{N}M)^{2}d\Omega^{2}$$
$$= -\rho^{2}d\tau^{2} + \rho^{2} + (2G_{N}M)^{2}d\Omega^{2},$$
(3.27)

where we have used $d\tau = \frac{1}{4G_{\rm N}M}dt$ in the last equation. This is just the Rindler metric! This makes sense because a stationary observer just outside the horizon must accelerate strongly to remain stationary.

In a quantum state that plays a similar role for the Schwarzschild geometry as the Minkowski space vacuum for the Rindler wedge, the accelerated observer outside the horizon should see a locally thermal state with temperature

$$T(r) = \frac{1}{2\pi\rho} = \frac{1}{4\pi\sqrt{2G_{\rm N}M(r - 2G_{\rm N}M)}},$$
(3.28)

in close analogy to the Unruh effect.

If one goes further away from the horizon, the temperature is red-shifted according to the metric (3.25) (excitations loose frequency when propagating up the gravitational potential) and one has

$$T(r') = \frac{1}{4\pi\sqrt{2G_{\rm N}M(r - 2G_{\rm N}M)}} \frac{\sqrt{1 - \frac{2G_{\rm N}M}{r}}}{\sqrt{1 - \frac{2G_{\rm N}M}{r'}}} = \frac{1}{4\pi\sqrt{2G_{\rm N}Mr\left(1 - \frac{2G_{\rm N}M}{r'}\right)}}.$$
 (3.29)

For $r' \to \infty$ and radius r close to the horizon $r \to 2G_{\rm N}M$ this becomes (in the last equation we restore SI units for clarity)

$$T_H = \frac{1}{8\pi G_{\rm N} M} = \frac{\hbar c^3}{8\pi G_{\rm N} M k_{\rm B}}.$$
 (3.30)

This is the *Hawking temperature* of a Schwarzschild black hole.

From the temperature it is straight forward to obtain an entropy by thermodynamic considerations. Consider the differential

$$dS = \frac{1}{T}dE = 8\pi G_{\rm N}MdE. \tag{3.31}$$

If some energy is added to the black hole it should increase in mass, dE = dM, so

$$dS = 8\pi G_{\rm N} M dM = 4\pi G_{\rm N} d(M^2). \tag{3.32}$$

Assuming S=0 for M=0 one can integrate this to $S=4\pi G_{\rm N}M^2$. Moreover, the result can be written in terms of the area of the horizon $A=4\pi R^2=4\pi(2G_{\rm N}M)^2$ and one obtains

$$S = \frac{A}{4G_{\rm N}} = \frac{A}{4l_p^2} = \frac{Ac^3k_{\rm B}}{4\hbar G_{\rm N}},\tag{3.33}$$

where we have used the Planck length $l_p = \sqrt{G_N \hbar/c^3}$ and restored SI units for clarity in the last equation. The result (3.33) is known as the *Bekenstein-Hawking entropy* of a Schwarzschild black hole.

It is currently unclear whether the Bekenstein-Hawking entropy can also be derived directly an an entanglement or relative entanglement entropy.

3.7 Modular hamiltonian for conformal field theory in double-light cone geometry

For conformal field theories, the entanglement or modular Hamiltonian is also known for another geometry, namely a region in Minkowski space bounded by two light cones [19, 20] (see also [21]).

Consider a light cone originating at a point p^{μ} in d-dimensional Minkowski space and another one ending at the point q^{μ} in the future of p^{μ} (see figure 2 for an illustration). The two light cones intersect on a ball of dimension d-2 (i. e. two points for d=1+1 and a surface in d=3+1). One may now consider any hypersurface in the interior of the double light cone region with boundary on the intersection of the two light cones. One can then write the reduced density matrix in that region as

$$\rho = \frac{1}{Z}e^{-K}, \qquad Z = \text{Tr } e^{-K},$$
(3.34)

where K is given by the local expression

$$K = \int_{\Sigma} d\Sigma_{\mu} \, \xi_{\nu}(x) T^{\mu\nu}(x) \,. \tag{3.35}$$

Here $T^{\mu\nu}(x)$ is again the energy-momentum tensor of excitations in the field theory and $\xi^{\nu}(x)$ is a vector field that can be written as

$$\xi^{\mu}(x) = \frac{2\pi}{(q-p)^2} \left[(q-x)^{\mu}(x-p)(q-p) + (x-p)^{\mu}(q-x)(q-p) - (q-p)^{\mu}(x-p)(q-x) \right]. \tag{3.36}$$

Note that (3.35) is again of the same form as a density matrix of a thermal state if one identifies $\xi^{\mu} = \frac{1}{T}u^{\mu}$ the vector of (inverse of) temperature T and fluid velocity u^{μ} . The vector ξ^{μ} vanishes on the boundary of the region enclosed by the two light cones corresponding formally to an infinite temperature.

To repeat, the above result holds only for conformal field theories. This is also underlined by the fact that $\xi^{\mu}(x)$ in (3.36) is a conformal Killing vector field which satisfies (3.4) but not a Killing vector field as would be needed for a thermal equilibrium state of a non-conformal field theory.

In d = 1 + 1 dimensions, one can obtain the modular Hamiltonian for the Rindler wedge from the double light cone region by sending one light-cone intersection point to spatial infinity. There is another interesting limit which corresponds to the early-time limit of an expanding quantum string; this will be discussed below.

3.8 Entanglement in an expanding quantum string

Consider a region in d=1+1 dimension bound by a light cone originating at t=x=0. This is the region of particle production from an expanding QCD string that forms between a highly energetic quark-anti-quark pair produced at t=x=0 (e.g. from a virtual photon in e^+e^- collisions). One can send the end point of the future light cone q to time-like infinity, and (3.35) assumes a relatively simple form. This is best described in terms of Bjorken (or Milne) coordinates of proper time τ and rapidity η related to standard Minkowski space coordinates by

$$t = \tau \cosh(\eta), \qquad z = \tau \sinh(\eta).$$
 (3.37)

In this coordinates, the limit of (3.36) is a vector $\beta^{\mu} = u^{\mu}/T$ where u^{μ} points in the direction of translations in Bjorken time τ and the temperature reads (in the second equation we restore SI units for clarity)

$$T(\tau) = \frac{1}{2\pi\tau} = \frac{\hbar}{2\pi\tau k_{\rm B}}.\tag{3.38}$$

This time dependent entanglement temperature governs the early time limit of an expanding quantum string [5, 22]. In fact, a QCD-type string is not conformal baut at very early proper time τ , there is an emerging conformal symmetry when the one-dimensional "Hubble rate" $H=1/\tau$ is much larger than any other relevant mass scale.

One can show that this temperature is indeed a result of entanglement between different regions in Minkowski space. Finite regions in Minkowski space have reduced density matrices that describe mixed states (as a result of entanglement). For a massive field theory, one can consider a rapidity interval $\Delta \eta$ at fixed dimensionless combination $M\tau$. If one takes $\Delta \eta \to \infty$ for fixed $M\tau$, one recovers formally a pure state with vanishing entanglement per unit rapidity, $\partial S_{\Delta\eta}/\partial \Delta \eta \to 0$. In contrast, if one first takes the conformal limit $M\tau \to 0$ and then $\Delta \eta \to \infty$, one finds formally a mixed state with finite entanglement entropy per unit rapidity $\partial S_{\Delta\eta}/\partial \Delta \eta \to c/6$ and non-zero temperature $T = 1/(2\pi\tau)$ [5, 22].

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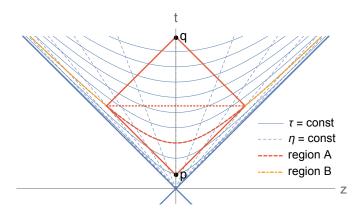


Figure 2: Illustration of Bjorken coordinates and causal development of a rapidity interval $(-\Delta\eta/2, \Delta\eta/2)$ at fixed proper time τ (region A, dashed red line). The complement region B corresponds to $(-\infty, -\Delta\eta/2)$ and $(\Delta\eta/2, \infty)$ (dot-dashed orange line). The point p is the origin of the past light cone that delimits region A and q is the endpoint of the future light cone. For better orientation we also show lines of constant proper time τ and rapidity η .

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