Entropy for Gaussian states

The aim of this problem is to obtain the formula for entropy of bosonic Gaussian states in terms of correlators. Gaussian states arise naturaly as fundamental states or thermal equilibrium states for quadratic bosonic or fermionic Hamiltonians. For Bosonic systems the Hilbert space is infinite dimensional, while for N fermions the dimension is 2^N. However, in both cases you will find the entropy is given in terms of eigenvalues of a $N \times N$ matrix. This simplification is due to the particularly simple structure of correlators for these states.

Let the Hermitian operators ϕ_i and π_j (coordinate and conjugate momentum bosonic operators) obey the canonical commutation relations

$$[\phi_i, \pi_j] = i\delta_{ij}\,, \qquad [\phi_i, \phi_j] = [\pi_i, \pi_j] = 0\,. \tag{1}$$

This forms a canonical commutation algebra. A Gaussian state is a state such that all non-zero correlators are obtained from the two point correlators by the prescription

$$\langle f_1 f_2 ... f_{2k} \rangle = \frac{1}{2^k k!} \sum_\sigma \left\langle \mathcal{O} f_{\sigma(1)} f_{\sigma(2)} \right\rangle ... \left\langle \mathcal{O} f_{\sigma(2k-1)} f_{\sigma(2k)} \right\rangle\,, \tag{2}$$

where the sum is over all the permutations σ of the indices, the f_i can be any of the field or momentum variables, and $\mathcal{O}$ means the ordering of the operators in the two point correlators has to be the same as the ordering they have in the left hand side of the equation. More simply, a state is Gaussian if a $2n$-point correlator is a sum over all possible products of two point correlators that can be formed with the $2n$ operators, each of these products taken with multiplicity one, and mantaining the ordering of the variables. For example

$$\langle f_1 f_2 f_3 f_4 \rangle = \langle f_1 f_2 \rangle \langle f_3 f_4 \rangle + \langle f_1 f_3 \rangle \langle f_2 f_4 \rangle + \langle f_1 f_4 \rangle \langle f_2 f_3 \rangle\,. \tag{3}$$

We are assuming that $\langle \phi \rangle = \langle \pi \rangle = 0$, and expectation values of products of an odd number of canonical variables vanish as well[1]. A Gaussian state is also called "free" or "quasifree", and the property (2) is a consequence of Wick's theorem for vacuum state of free fields. As we will see a Gaussian state can be pure or mixed.

a) Convince yourself this property is compatible with the numerical commutation relations for the canonical variables. Convince yourself that if the state is Gaussian for the $2N$ operators ϕ_i, π_i, it will be also Gaussian for arbitrary linear combinations of these operators.

b) The two point functions can be written as

$$\langle \phi_i \phi_j \rangle = X_{ij}\,, \qquad \langle \pi_i \pi_j \rangle = P_{ij}\,, \tag{4}$$

$$\langle \phi_i \pi_j \rangle = \langle \pi_j \phi_i \rangle^* = \frac{i}{2}\delta_{ij} + D_{ij}\,, \tag{5}$$

Show X and P are real, Hermitian, positive definite, and D is real. From now on we will restrict attention to this case with $D_{ij} = 0$ (this corresponds to time inversion symmetry of the state).

c) By definition the reduced density matrix is the unique matrix that satisfies

$$\langle O \rangle = \mathrm{tr}(\rho O)\,, \tag{6}$$

for any operator O, that is, any function of ϕ_i, π_i, which we can think can be approximated by polynomials in these variables. Hence, the reduced density matrix must be such that expectation values give the right two point functions and Wick's theorem for the canonical variables.

Propose the following anzats for the reduced density matrix

$$\rho = K e^{-\mathcal{H}} = K\, e^{-\Sigma \epsilon_l a_l^\dagger a_l}\,, \tag{7}$$

[1] The case of non vanishing one point functions is a simple generalization.

in terms of independent creation and annihilation operators

$$[a_i, a_j^\dagger] = \delta_{ij}\,, \tag{8}$$

which are expressed as (at this moment undetermined) linear combinations of the ϕ_i and π_j,

$$\begin{aligned} \phi_i &= \alpha_{ij} a_j^\dagger + \alpha_{ij} a_j\,, && (9)\\ \pi_i &= -i\beta_{ij} a_j^\dagger + i\beta_{ij} a_j\,. && (10) \end{aligned}$$

Here α and β are real matrices. General linear transformations of bosonic operators are called Bogoliubov transformations.

Note that (7) gives the reduced density matrices as a product of independent density matrices for oscillators with mode annihilation operators a_i, and that the state on each of these independent modes is a thermal state for a harmonic oscillator. Compute the normalization constant K. What is the spectrum of this density matrix? Compute the entropy of the density matrix (7) in terms of the ϵ_k.

d) As a first step in showing the anzats (7) gives the correct state, argue that this state satisfies Wick's theorem for the operators a_i, $a_j^\dagger$. Then use the fact that if Wick's theorem holds for certain variables it will hold for linear combinations of the variables. In this way we know that the state (7) satisfies Wick's theorem for the original ϕ_i, π_j variables. It only remain to choose the Bogoliubov transformation such that the two point correlators match.

e) Show that in order that transformations (9), (10) satisfy the canonical commutation relations we have

$$\alpha\beta^T = -\frac{1}{2}\,. \tag{11}$$

f) Compute the two point correlation functions from (6), using $\mathrm{tr}(\rho\phi_i\phi_j) = X_{ij}$, $\mathrm{tr}(\rho\pi_i\pi_j) = P_{ij}$, to obtain the matrix equations

$$\begin{aligned} \alpha(2n+1)\alpha^T &= X\,, && (12)\\ \beta(2n+1)\beta^T &= P\,, && (13) \end{aligned}$$

where n is the diagonal matrix of the expectation value of the occupation number

$$n_{kk} = \left\langle a_k^\dagger a_k \right\rangle = (e^{\epsilon_k} - 1)^{-1}\,. \tag{14}$$

g) These equations give

$$\alpha\frac{1}{4}(2n+1)^2\alpha^{-1} = XP\,. \tag{15}$$

This last equation gives the spectrum ϵ_k of the independent oscillators in terms of the spectrum of XP,

$$(1/2)\coth(\epsilon_k/2) = \nu_k\,, \tag{16}$$

where ν_k are the (positive) eigenvalues of

$$C = \sqrt{XP}\,. \tag{17}$$

Using this relation between eigenvalues, rewrite the entropy in terms of the matric C as:

$$S = \mathrm{tr}\left((C+1/2)\log(C+1/2) - (C-1/2)\log(C-1/2)\right)\,. \tag{18}$$

This is the expression we were looking for. What is the analogous expression for the Renyi entropies? You can also compute the modular Hamiltonian in terms of X and P.

h) The expression (18) for the entropy requires the eigenvalues of C to be greater than 1/2 or the eigenvalues of $X.P$ are greater than 1/4. Can you explain why this inequality for the correlators is always true? If the state is pure derive a relation the correlators X and P have to satisfy.

i) The fundamental state (vacuum) of a quadratic Hamiltonian of the form

$$H = \frac{1}{2}\sum \pi_i^2 + \frac{1}{2}\sum_{ij} \phi_i K_{ij} \phi_j \,, \tag{19}$$

is a Gaussian state[2]. Show the two point correlators are given by

$$\begin{aligned} X_{ij} &= \langle \phi_i \phi_j \rangle = \frac{1}{2}(K^{-\frac{1}{2}})_{ij} \,, && (20)\\ P_{ij} &= \langle \pi_i \pi_j \rangle = \frac{1}{2}(K^{\frac{1}{2}})_{ij} \,, && (21)\\ D_{ij} &= 0 \,. && (22) \end{aligned}$$

Now, if we want to study the vacuum state reduced to a subset V (a "region") of degrees of freedom given by some pairs ϕ_i, π_i, $i \in V$, of the original variables, it is an inmediate observation that the reduced state will continue to be Gaussian for the correlators restricted to V. Hence, we can use the correlators (20) and (21), but with matrix indices restricted to V, and compute the entropy with formula (18) using these restricted matrices. Note that the only information that we need is the Hamiltonian (the matrix K). What is the entropy for the global fundamental state according to (18) and (20), (21)?

A similar calculation can be done for fermion Gaussian states. See the original reference I. Peschel, J. Phys. A: Math. Gen. 36, L205 (2003), arXiv:cond-mat/0212631, or the review H. Casini, M. Huerta, J.Phys. A42 (2009) 504007, arXiv:0905.2562. See H. Casini, M. Huerta, Phys.Rev. D93 (2016) 105031, arXiv:1406.2991, for Gaussian gauge fields. The method can also be applied to other, non vacuum, Gaussian states, such as thermal states or states with chemical potential for free fermions or bosons, and some states in curved space for non interacting fields. Note that there are many states for a free theory that are not Gaussian.

[2] You can think the vacuum state is the zero temperature limit of the thermal state. A thermal state is an exponential of the Hamiltonian, and you have shown that states which are exponentials of quadratic operators are Gaussian.