

Monotonicity of Relative Entropy In Quantum Field Theory

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The goal of this lecture is to explain two things:

- (1) The Reeh-Schlieder theorem (1961), which is the basic result showing that entanglement is unavoidable in quantum field theory.
- (2) A very specific version of monotonicity of relative entropy in quantum field theory: relative entropy is monotonic under decreasing the size of a region.

The second statement was used by A. Wall in proving a generalized second law of thermodynamics in the presence of a black hole.

If one is familiar with the proof of this second statement, it is not too difficult to understand the general proof of strong subadditivity of quantum entropy (which has had many additional applications) and its close cousin, monotonicity of entropy in a general quantum channel, but we will not have time for this. (This and many related matters are described in my article “Notes On Some Entanglement Properties Of Quantum Field Theory,” on the arXiv.)

We begin with the Reeh-Schlieder theorem, which must have seemed paradoxical when it was first discovered in 1961. We consider a quantum field theory in Minkowski spacetime M , with a Hilbert space \mathcal{H} that contains a vacuum state Ω . There is an algebra of local operators, whose action can produce “all” states (or at least all states in a superselection sector) from the vacuum. For simplicity in the notation, we will assume that this operator algebra is generated by a hermitian scalar field $\phi(x)$. So states

$$\phi(x_1)\phi(x_2)\cdots\phi(x_n)|\Omega\rangle$$

with arbitrary n and points $x_1, \dots, x_n \in M$, are dense in \mathcal{H} .

The Reeh-Schlieder theorem says that actually, we get a dense set of states (in the vacuum sector of \mathcal{H}) if we restrict the points x_1, \dots, x_n to any possibly very small open set $\mathcal{U} \subset M$:

M



If this is false, there is a state χ in the vacuum sector such that

$$\langle \chi | \phi(x_1) \phi(x_2) \cdots \phi(x_n) | \Omega \rangle = 0$$

whenever $x_1, \dots, x_n \in \mathcal{U}$.

We will show that any such χ actually satisfies

$$\langle \chi | \phi(x_1) \phi(x_2) \cdots \phi(x_n) | \Omega \rangle = 0$$

for all $x_i \in M$. Since states created by the ϕ 's are dense (in the vacuum sector) this implies that $\chi = 0$.

Let us define

$$f(x_1, x_2, \cdots, x_n) = \langle \chi | \phi(x_1) \phi(x_2) \cdots \phi(x_n) | \Omega \rangle.$$

We are given that this function vanishes if the x_i are in \mathcal{U} and we want to prove that it vanishes for all x_i .

As a first step, pick a future-pointing timelike vector t and consider shifting x_n by a real multiple of t :

$$x_n \rightarrow x_n + ut.$$

Let

$$g(u) = \langle \chi | \phi(x_1) \phi(x_2) \cdots \phi(x_{n-1}) \phi(x_n + ut) | \Omega \rangle$$

with $x_i \in \mathcal{U}$. We have $g(u) = 0$ for sufficiently small real u because then $x_n + ut$ is still in u . Also with H the Hamiltonian for translation in the t direction,

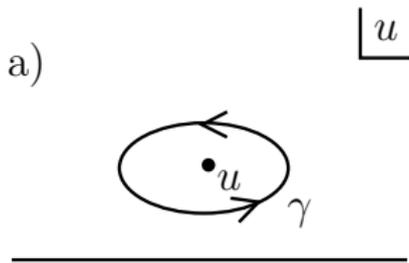
$$g(u) = \langle \chi | \phi(x_1) \phi(x_2) \cdots \exp(iHu) \phi(x_n) \exp(-iHu) | \Omega \rangle.$$

Since $H\Omega = 0$ this is

$$g(u) = \langle \chi | \phi(x_1) \phi(x_2) \cdots \exp(iHu) \phi(x_n) | \Omega \rangle$$

and since H is nonnegative, $g(u)$ is holomorphic in the upper half u -plane.

Such a function is zero. If we knew $g(u)$ to be holomorphic *on* the real axis and vanishing on a segment I of the real axis, we would say that $g(u)$ has a convergent Taylor series expansion around a point $p \in I$ and this expansion would have to be identically zero to make $g(u)$ vanish on the axis. To begin with we only know that $g(u)$ is holomorphic above the real axis, not on it, but we can get around this using the Cauchy integral formula:



So now we know that (keeping $x_1, \dots, x_{n-1} \in \mathcal{U}$)

$$\langle \chi | \phi(x_1) \cdots \phi(x_{n-1}) \phi(x'_n) | \Omega \rangle$$

vanishes if $x'_n = x_n + ut$ where t is a timelike vector and u is any real number. Now we do this again, picking another timelike vector t' and replacing x'_n by $x''_n = x'_n + u't'$ with u' real. Repeating the argument, we learn that

$$\langle \chi | \phi(x_1) \cdots \phi(x_{n-1}) \phi(x''_n) | \Omega \rangle = 0$$

for any such x''_n . But since any point in M can be reached from \mathcal{U} by zigzagging backwards and forwards in various timelike directions, we learn that

$$\langle \chi | \phi(x_1) \cdots \phi(x_{n-1}) \phi(x_n) | \Omega \rangle = 0$$

for $x_1, \dots, x_{n-1} \in \mathcal{U}$ with no restriction on x_n .

The next step is to remove the restriction on x_{n-1} . We pick t as before and now consider a common shift of x_{n-1} and x_n in the t direction

$$(x_{n-1}, x_n) \rightarrow (x'_{n-1}, x'_n) = (x_{n-1} + ut, x_n + ut)$$

Now we look at

$$h(u) = \langle \chi | \phi(x_1) \phi(x_2) \cdots \phi(x_{n-1} + ut) \phi(x_n + ut) | \Omega \rangle$$

It vanishes for small real u , and it can be written

$$h(u) = \langle \chi | \phi(x_1) \phi(x_2) \cdots \exp(iuH) \phi(x_{n-1}) \phi(x_n) | \Omega \rangle,$$

which implies that $h(u)$ is holomorphic in the upper half plane. Hence $h(u)$ is identically 0.

Repeating the process by shifting x_{n-1} and x_n in some other timelike direction, we learn that

$$\langle \chi | \phi(x_1) \cdots \phi(x_{n-1}) \phi(x_n) | \Omega \rangle$$

vanishes for $x_1, \dots, x_{n-2} \in \mathcal{U}$ with no restriction on x_{n-1}, x_n . The next step is to remove the restriction on x_{n-2} . We do this in exactly the same way, by considering what happens when we shift the last three coordinates by a common timelike vector. And so on.

So we end up proving the Reeh-Schlieder theorem: an “arbitrary” state (more exactly, a dense set of states in the vacuum sector of Hilbert space) can be created from the vacuum by acting with a product of local operators in a small open set $\mathcal{U} \subset M$.

Now I want to discuss the interpretation of this theorem. The first question that I want to dispose of is whether it contradicts causality. It certainly sounds unintuitive at first sight. Consider a state of the universe that on some initial time slice looks like the vacuum near \mathcal{U} , but contains the planet Jupiter at a distant region spacelike \mathcal{V} separated from \mathcal{U} . Let J be a “Jupiter” operator whose expectation value in a state that contains the planet Jupiter in region \mathcal{V} is close to 1, while its expectation value is close to 0 otherwise. The Reeh-Schlieder theorem says that there is an operator X in region \mathcal{U} such that the state $X\Omega$ contains the planet Jupiter in region \mathcal{V} . So

$$\langle \Omega | J | \Omega \rangle \cong 0, \quad \langle X\Omega | J | X\Omega \rangle \cong 1.$$

Is this a contradiction? Since X is supported in \mathcal{U} and J in the spacelike separated region \mathcal{V} , X^\dagger and J commute. So

$$1 \cong \langle X\Omega | J | X\Omega \rangle = \langle \Omega | X^\dagger J X | \Omega \rangle = \langle \Omega | J X^\dagger X | \Omega \rangle.$$

If X were *unitary* there would be a contradiction between the statements

$$0 \cong \langle \Omega | J | \Omega \rangle$$

and

$$1 \cong \langle \Omega | J X^\dagger X | \Omega \rangle,$$

because if X is unitary, then $X^\dagger X = 1$. But the Reeh-Schlieder theorem does not tell us that we can pick X to be unitary; it just tells us that there is *some* X in region \mathcal{U} that will create the planet Jupiter in a distant region \mathcal{V} .

In comparing the above formulas, all we have found is that in the vacuum, the operators J and $X^\dagger X$ have a nonzero correlation function in the vacuum at spacelike separation. There is no contradiction there; spacelike correlations in quantum field theory are ubiquitous, even in free field theory.

The intuitive interpretation of the Reeh-Schlieder theorem involves entanglement between the degrees of freedom inside an open set \mathcal{U} and those at spacelike separation from \mathcal{U} . To explain the intuitive picture, let us imagine that the Hilbert space \mathcal{H} of our QFT has a factorization

$$\mathcal{H} = \mathcal{H}_{\mathcal{U}} \otimes \mathcal{H}_{\mathcal{U}'}$$

where $\mathcal{H}_{\mathcal{U}}$ describes the degrees of freedom in region \mathcal{U} and $\mathcal{H}_{\mathcal{U}'}$ describes all of the degrees of freedom outside of \mathcal{U} . Then any state in \mathcal{H} , such as the vacuum state Ω , would have a decomposition

$$\Omega = \sum_i \sqrt{p_i} \psi_{\mathcal{U}}^i \otimes \psi_{\mathcal{U}'}^i$$

where we can assume the states $\psi_{\mathcal{U}}^i$ and also $\psi_{\mathcal{U}'}^i$ to be orthonormal and we assume the p_i are all positive (otherwise we drop some terms from the sum).

In general when we write

$$\Omega = \sum_i \sqrt{p_i} \psi_{\mathcal{U}}^i \otimes \psi_{\mathcal{U}'}^i$$

the $\psi_{\mathcal{U}}^i$ and $\psi_{\mathcal{U}'}^i$ do not form a basis of $\mathcal{H}_{\mathcal{U}}$ or of $\mathcal{H}_{\mathcal{U}'}$, because there are not enough of them. However, something like the Reeh-Schlieder theorem will be true for any state Ω such that the $\psi_{\mathcal{U}}^i$ and the $\psi_{\mathcal{U}'}^i$ do form bases of their respective spaces. Using the fact that the $\psi_{\mathcal{U}'}^i$ are a basis of $\mathcal{H}_{\mathcal{U}'}$, we would be able to expand any state $\Psi \in \mathcal{H}$ as

$$\Psi = \sum_i \lambda_{\mathcal{U}}^i \otimes \psi_{\mathcal{U}'}^i, \quad \lambda^i \in \mathcal{H}_{\mathcal{U}}.$$

Then because the $\psi_{\mathcal{U}}^i$ are a basis and the p_i are nonzero, we can define a linear operator X acting on $\mathcal{H}_{\mathcal{U}}$ by

$$X(\sqrt{p_i} \psi_{\mathcal{U}}^i) = \lambda^i$$

and we see that we have found an operator X acting only on degrees of freedom in \mathcal{U} such that

$$X\Omega = \Psi.$$

A state

$$\Omega = \sum_i \sqrt{p_i} \psi_{\mathcal{U}}^i \otimes \psi_{\mathcal{U}'}^i$$

where the p_i are all positive and the $\psi_{\mathcal{U}}^i, \psi_{\mathcal{U}'}^i$ are bases might be called a “fully” entangled state. (I don’t think this is standard terminology.) We call a state “maximally” entangled if the p_i are all equal (this is not possible for Hilbert spaces of infinite dimension, as in quantum field theory). The Reeh-Schlieder theorem means intuitively that the vacuum state Ω of a quantum field theory is fully entangled in this sense, between the inside and outside of an arbitrary open set \mathcal{U} .

However, the decomposition

$$\mathcal{H} = \mathcal{H}_{\mathcal{U}} \otimes \mathcal{H}_{\mathcal{U}'}$$

that we started with is certainly not literally valid in quantum field theory. If it were, then in \mathcal{H} there would be an unentangled pure state $\psi \otimes \chi$, $\psi \in \mathcal{H}_{\mathcal{U}}$, $\chi \in \mathcal{H}_{\mathcal{U}'}$. This contradicts the fact that in quantum field theory there is a universal ultraviolet divergence in the entanglement entropy: the entanglement entropy of the vacuum between degrees of freedom in \mathcal{U} and those outside of \mathcal{U} is ultraviolet divergent, and the leading ultraviolet divergence is universal, that is it is the same for any state. The leading divergence is universal because any state looks like the vacuum at short distances.

Now let us discuss an important corollary of the Reeh-Schlieder theorem. Let \mathcal{U} and \mathcal{V} be spacelike separated open sets in Minkowski spacetime:



Let b be an operator supported in \mathcal{V} . Suppose that

$$b\Omega = 0.$$

Then if a is supported in \mathcal{U} , we have

$$b(a\Omega) = ab\Omega = 0,$$

where I use the fact that $[a, b] = 0$ since \mathcal{U} and \mathcal{V} are spacelike separated. But the states $a\Omega$ are dense in \mathcal{H} (according to Reeh-Schlieder) so b identically vanishes.

Thus if $b \neq 0$ is supported in a spacelike open set \mathcal{V} that is small enough that it is spacelike separated from another open set \mathcal{U} , then

$$b\Omega \neq 0.$$

The roles of \mathcal{U} and \mathcal{V} are symmetrical, so also for $a \neq 0$ supported in \mathcal{U} ,

$$a\Omega \neq 0.$$

Let $\mathcal{A}_{\mathcal{U}}$ be the algebra of operators in region \mathcal{U} . We have proved two facts about the algebra $\mathcal{A}_{\mathcal{U}}$ acting on the vacuum sector \mathcal{H} :

(1) States $a\Omega$, $a \in \mathcal{A}_{\mathcal{U}}$, are dense in \mathcal{H} . This is described by saying that Ω is a “cyclic” vector for the algebra $\mathcal{A}_{\mathcal{U}}$.

(2) For any nonzero $a \in \mathcal{A}_{\mathcal{U}}$, $a\Omega \neq 0$. This is described by saying that Ω is a “separating” vector of $\mathcal{A}_{\mathcal{U}}$.

In short, the Reeh-Schlieder theorem and its corollary say that the vacuum is a cyclic separating vector for $\mathcal{A}_{\mathcal{U}}$.

Consider a quantum system with a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ and let \mathcal{A} be the algebra of operators on \mathcal{H}_1 . A little thought shows that a general vector Ψ expanded in the usual way

$$\Psi = \sum_i \sqrt{p_i} \psi_1^i \otimes \psi_2^i$$

is cyclic for \mathcal{A} if the ψ_2^i are a basis of \mathcal{H}_2 , and it is separating for \mathcal{A} if the ψ_1^i are a basis for \mathcal{H}_1 . So that is the meaning of the cyclic separating property if the Hilbert space is a tensor product.

What about quantum field theory? A mathematical machinery that can be useful for analyzing entanglement when the Hilbert space does not factorize is called Tomita-Takesaki theory. It applies whenever one has an algebra \mathcal{A} acting on a Hilbert space \mathcal{H} with a cyclic separating vector.

The starting point in Tomita-Takesaki theory is that, given an algebra \mathcal{A} with cyclic separating vector Ψ , we define an antilinear operator

$$S_{\Psi} : \mathcal{H} \rightarrow \mathcal{H}$$

by

$$S_{\Psi} a \Psi = a^{\dagger} \Psi.$$

The definition makes sense because of the separating property (if we could have $a \Psi = 0$ with $a^{\dagger} \Psi \neq 0$, we would get a contradiction) and it does define S_{Ψ} on a dense set of states in \mathcal{H} , because of the cyclic property (states $a \Psi$ are dense in \mathcal{H}). A couple of obvious facts are that

$$S_{\Psi}^2 = 1$$

(which in particular says that S_{Ψ} is invertible) and

$$S_{\Psi} |\Psi\rangle = |\Psi\rangle.$$

The *modular operator* is a linear, self-adjoint operator defined by

$$\Delta_\Psi = S_\Psi^\dagger S_\Psi.$$

(The definition of the adjoint of an antilinear operator is $\langle \alpha | S | \beta \rangle = \langle \beta | S^\dagger | \alpha \rangle$.) Δ_Ψ is positive-definite because S_Ψ is invertible.

We will also need the relative modular operator. Let the state Ψ be cyclic separating, and let Φ be any other state. The relative modular operator $S_{\Psi|\Phi}$ is an antilinear operator defined by

$$S_{\Psi|\Phi} a |\Psi\rangle = a^\dagger |\Phi\rangle.$$

Again the well-definedness of the definition depends on the cyclic separating nature of Ψ , but no property of Φ is needed. In defining $S_{\Psi|\Phi}$, we assume that Ψ and Φ are unit vectors

$$\langle \Psi | \Psi \rangle = \langle \Phi | \Phi \rangle = 1.$$

The relative modular operator is defined by

$$\Delta_{\Psi|\Phi} = S_{\Psi|\Phi}^\dagger S_{\Psi|\Phi}.$$

It is still self-adjoint and positive semi-definite, but it is not necessarily invertible. If $\Phi = \Psi$ then the definitions reduce to the previous ones

$$S_{\Psi|\Psi} = S_\Psi, \quad \Delta_{\Psi|\Psi} = \Delta_\Psi.$$

Now we are ready to define relative entropy in quantum field theory. We fix an open set \mathcal{U} (small enough so that the vacuum is cyclic separating), and consider the algebra $\mathcal{A}_{\mathcal{U}}$. Let Ψ be any cyclic separating vector for $\mathcal{A}_{\mathcal{U}}$, and Φ any other vector. The relative entropy between the states Ψ and Φ , for measurements in region \mathcal{U} (as defined by Araki in the 1970's) is

$$S_{\Psi|\Phi}(\mathcal{U}) = -\langle \Psi | \log \Delta_{\Psi|\Phi} | \Psi \rangle.$$

It is not immediately obvious that this has anything to do with relative entropy as defined for a general quantum system (and as used for example in Casini's proof of the Bekenstein bound), but it is not hard to show that the definitions coincide. (The main step in doing this is to understand the operators $S_{\Psi|\Phi}$ and $\Delta_{\Psi|\Phi}$ when the Hilbert space does factorize. See for example section 4 of my notes.)

First let us discuss positivity properties of relative entropy, defined by

$$\mathcal{S}_{\Psi|\Phi}(\mathcal{U}) = -\langle \Psi | \log \Delta_{\Psi|\Phi} | \Psi \rangle.$$

First of all, if $\Phi = \Psi$ then we had

$$\Delta_{\Psi}\Psi = \Psi$$

so

$$(\log \Delta_{\Psi})\Psi = 0$$

and hence the relative entropy between Ψ and itself is 0:

$$\mathcal{S}_{\Psi|\Psi}(\mathcal{U}) = 0.$$

But more than that, suppose that $\Phi = a'\Psi$, where a' is unitary and $[a', \mathcal{A}_{\mathcal{U}}] = 0$, so that measurements in region \mathcal{U} cannot distinguish Φ from Ψ . A short computation shows that in this case $\Delta_{\Psi|\Phi} = \Delta_{\Psi}$ so again

$$\mathcal{S}_{\Psi|a'\Psi}(\mathcal{U}) = 0.$$

Now consider a completely general state Φ . The inequality $-\log \lambda \geq 1 - \lambda$ for a positive real number λ implies an operator inequality $-\log \Delta \geq 1 - \Delta$, implying

$$\begin{aligned} \mathcal{S}_{\Psi|\Phi}(\mathcal{U}) &= -\langle \Psi | \log \Delta_{\Psi|\Phi} | \Psi \rangle \geq \langle \Psi | (1 - \Delta_{\Psi|\Phi}) | \Psi \rangle \\ &= \langle \Psi | \Psi \rangle - \langle \Psi | S_{\Psi|\Phi}^\dagger S_{\Psi|\Phi} | \Psi \rangle = \langle \Psi | \Psi \rangle - \langle \Phi | \Phi \rangle = 0. \end{aligned}$$

So in general

$$\mathcal{S}_{\Psi|\Phi}(\mathcal{U}) \geq 0.$$

Now we consider a smaller open set $\tilde{\mathcal{U}} \subset \mathcal{U}$. Now we have two different algebras $\mathcal{A}_{\tilde{\mathcal{U}}} \subset \mathcal{A}_{\mathcal{U}}$ and two different operators $S_{\Psi|\Phi;\tilde{\mathcal{U}}}$ and $S_{\Psi|\Phi;\mathcal{U}}$ and associated modular operators $\Delta_{\Psi|\Phi;\tilde{\mathcal{U}}}$ and $\Delta_{\Psi|\Phi;\mathcal{U}}$. The relative entropy between Ψ and Φ for measurements in \mathcal{U} is

$$\mathcal{S}_{\Psi|\Phi}(\mathcal{U}) = -\langle \Psi | \log \Delta_{\Psi|\Phi;\mathcal{U}} | \Psi \rangle.$$

The corresponding relative entropy for measurements in $\tilde{\mathcal{U}}$ is

$$\mathcal{S}_{\Psi|\Phi}(\tilde{\mathcal{U}}) = -\langle \Psi | \log \Delta_{\Psi|\Phi;\tilde{\mathcal{U}}} | \Psi \rangle.$$

We want to prove that relative entropy is monotonic under increasing the region considered:

$$\mathcal{S}_{\Psi|\Phi}(\tilde{\mathcal{U}}) \leq \mathcal{S}_{\Psi|\Phi}(\mathcal{U}).$$

This is an important statement for applications; I already mentioned its use by A. Wall in proving a generalized second law.

The states Ψ and Φ will be held fixed in this discussion, so to lighten the notation we will omit subscripts and denote the operators just as $S_{\mathcal{U}}$, $S_{\tilde{\mathcal{U}}}$ and likewise $\Delta_{\mathcal{U}}$ and $\Delta_{\tilde{\mathcal{U}}}$. The main point of the proof is to show that as an operator

$$\Delta_{\tilde{\mathcal{U}}} \geq \Delta_{\mathcal{U}}.$$

As I will explain in a moment, this implies

$$\log \Delta_{\tilde{\mathcal{U}}} \geq \log \Delta_{\mathcal{U}}. \quad (*)$$

The inequality we want

$$-\langle \Psi | \log \Delta_{\tilde{\mathcal{U}}} | \Psi \rangle \leq -\langle \Psi | \log \Delta_{\mathcal{U}} | \Psi \rangle$$

is just a matrix element of inequality (*) in the state Ψ .

To show that if P and Q are positive self-adjoint operators and

$$P \geq Q \quad (*)$$

then also

$$\log P \geq \log Q$$

let

$$R(t) = tP + (1 - t)Q$$

so (by virtue of $(*)$), R is an increasing function of t , in the sense that $\dot{R}(t) \geq 0$. We have

$$\log R(t) = \int_0^\infty ds \left(\frac{1}{s} - \frac{1}{s + R} \right).$$

So

$$\frac{d}{dt} \log R(t) = \int_0^\infty ds \frac{1}{s + R} \dot{R} \frac{1}{s + R}.$$

The integrand is positive since it is BAB with A, B positive ($A = \dot{R}$, $B = 1/(s + R)$), so the integral is positive and thus $\frac{d}{dt} \log R \geq 0$. Hence $R(1) \geq R(0)$ or

$$\log P \geq \log Q.$$

So monotonicity of relative entropy under increasing the region considered will follow from an inequality

$$\Delta_{\tilde{u}} \geq \Delta_u.$$

If we try to understand this inequality, we may get confused at first. We have

$$\Delta_{\tilde{u}} = S_{\tilde{u}}^\dagger S_{\tilde{u}}, \quad \Delta_u = S_u^\dagger S_u,$$

Here the two S 's were defined, naively, by the same formula

$$S_{\tilde{u}} a \Psi = a^\dagger \Phi, \quad S_u a \Psi = a^\dagger \Psi$$

with the sole difference that a is in $\mathcal{A}_{\tilde{u}}$ in one case and in \mathcal{A}_u in the other. The algebra \mathcal{A}_u is bigger, so S_u is defined on more states. But states $a\Psi$ with $a \in \mathcal{A}_{\tilde{u}}$ are already dense in Hilbert space so actually $S_{\tilde{u}}$ and S_u coincide on a dense set of states.

If one is careless, one might assume that two operators that agree on a dense subspace of Hilbert space actually coincide. This is not true, however, for unbounded operators such as $S_{\tilde{U}}$ and S_U . We have to remember that an unbounded operator is never defined on all states in Hilbert space, only (at most) on a dense subspace. The proper statement is that S_U is an extension of $S_{\tilde{U}}$, meaning that S_U is defined whenever $S_{\tilde{U}}$ is defined and, on states on which they are both defined, they coincide. In our problem, S_U is a proper extension, because there are states $a\Psi$, $a \in \mathcal{A}_U$, that are not of the form $a\Psi$, $a \in \mathcal{A}_{\tilde{U}}$. Anyway, the fact that S_U is an extension of $S_{\tilde{U}}$ implies, as a general Hilbert space statement, that

$$S_{\tilde{U}}^\dagger S_{\tilde{U}} \geq S_U^\dagger S_U,$$

which is what we need for monotonicity of relative entropy.

The intuitive idea of the inequality

$$S_{\tilde{U}}^\dagger S_{\tilde{U}} \geq S_U^\dagger S_U$$

is that the fact that $S_{\tilde{U}}$ is defined on fewer states than S_U is defined on corresponds to a constraint that has been placed on the states in the case of $S_{\tilde{U}}$, and this constraint raises the energy. I will give an analogy that aims to make this obvious. Instead of S_U , we will consider the exterior derivative d mapping zero-forms (functions) on a manifold M to 1-forms. But we will assume that M has a boundary N , and we will consider two different versions of the operator d .

The first will be the operator d acting on differentiable functions that are constrained to vanish on the boundary of X :

$$\widehat{d} : f(x_1, \dots, x_n) \rightarrow \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right), \quad f|_{\partial X} = 0.$$

We also consider the same operator d without the constraint that f vanishes on the boundary. Differentiable functions that vanish on the boundary are dense in Hilbert space, so \widehat{d} and d are each defined on a dense subspace of Hilbert space; moreover, obviously, d is an extension of \widehat{d} since it is defined whenever \widehat{d} is defined and they agree when they are both defined.

Associated to \hat{d} is the Dirichlet Laplacian

$$\hat{\Delta} = \hat{d}^\dagger \hat{d}$$

and associated in the same way to d is the Neumann Laplacian

$$\Delta = d^\dagger d.$$

Here $\hat{\Delta}$ and Δ are nonnegative operators that coincide on a dense set of states, but $\hat{\Delta}$ is more positive than Δ because of the constraint that the wavefunction should vanish on the boundary.

Indeed, Δ is associated to the energy function

$$\langle f|\Delta|f\rangle = \frac{1}{2} \int_M d^n x \sqrt{g} |df|^2$$

but to get $\widehat{\Delta}$ we should add a boundary term to the energy. In fact, we can consider a family of operators Δ_t , $0 \leq t \leq \infty$ associated to the energy function

$$\langle f|\Delta_t|f\rangle = \frac{1}{2} \int_M d^n x \sqrt{g} |df|^2 + t \int_N d^{n-1} x \sqrt{g} |f|^2.$$

Clearly the operator Δ_t is an increasing function of t . For $t = 0$, Δ_t is the Neumann Laplacian, and for $t \rightarrow \infty$, Δ_t goes over to the Dirichlet Laplacian $\widehat{\Delta}$.

So $\widehat{\Delta} \geq \Delta$, which is analogous to our desired $\Delta_{\tilde{u}} \geq \Delta_u$. A constraint on the state always raises the energy.

Just to make sure the analogy is clear, $\Delta_{\tilde{u}}$ is the operator associated to the energy function

$$\langle S_{\tilde{u}}\Lambda | S_{\tilde{u}}\Lambda \rangle$$

for a state Λ that should be in the domain of $S_{\tilde{u}}$. Δ_u is similarly associated to

$$\langle S_u\Lambda | S_u\Lambda \rangle$$

for a state Λ that should be in the larger domain of S_u . The second energy function is the same as the first except that it is defined on a larger space of states; we can get the second from the first by a constraint that removes some states. Such a constraint can only raise the energy so $\Delta_{\tilde{u}} \geq \Delta_u$. (The precise proof uses the projection onto the graph of an operator. See for example section 3.6 of my notes.)