

S-Theorem: Incompatibility of Scale Invariance and Hermiticity of Hamiltonian

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In this brief note, it has been shown that scale invariance (i.e the scaling algebra $[D, H] = izH$) is incompatible with Hamiltonian (H) being Hermitian on a domain containing the state $D|E\rangle$, where $|E\rangle$ is the non-zero energy eigenstate and D generates scale transformation. The claim has been elucidated with the strongly coupled regime of inverse square potential and the free particle as concrete examples. The proof presented can be generalised to the statement that any operator A having a definite scaling dimension, can not be Hermitian on a domain containing $D|A\rangle$ where $|A\rangle$ is the eigenstate of operator A . As a corollary, we find that classically scale invariant system can not be made quantum without losing either unitarity or scale invariance if we insist on having bound states with finite binding energy.

INTRODUCTION

Symmetries are holy grail of Physics. Symmetries are related to conserved quantities in a physical system due to Noether's theorem [1], which states that for every continuous symmetry, there is a conserved charge. Having a knowledge of conserved charges facilitates the study of physics of the system in concern. The symmetry can either be space-time symmetry i.e transformation on space-time that does not change the physical system under consideration or be an internal one acting on internal degrees of freedom associated with the system. For example, translational invariance is a space-time symmetry for which momentum is a conserved charge whereas conservation of quantities like electric charge are result of some internal symmetry.

In this note, we will focus on scaling symmetry, which is a space-time symmetry. Specifically, we will be interested in quantum implementation of scaling invariance i.e invariance under scaling transformation :

$$\vec{x} \rightarrow s\vec{x}, t \rightarrow s^z t \quad (0.1)$$

where z is the dynamical exponent of the system, allowing for systems which are invariant under different scaling of time and space. In relativistic systems, $z = 1$ due to Lorentz invariance. But in absence of Lorentz invariance, z can have any value. In quantum description of a scale invariant system, the Hamiltonian H and the generator of scale transformation D obeys the following commutation relation:

$$[D, H] = izH \quad (0.2)$$

We will show that (0.2) is incompatible with H being Hermitian on a domain containing the state $D|E\rangle$, where $|E\rangle$ is the non-zero energy eigenstate, henceforth called **S-Theorem**. S-Theorem can be used to deduce that classically scale invariant system can not be made quantum without losing either unitarity or scale invariance if we insist on having bound states with finite non-zero

binding energy.

We will elucidate our claim using two well studied examples, one of which is inverse square potential. This potential is a subject of study for long time, starting from [2]. It serves as a platform for simple realisation of quantum anomaly, where the classical scale symmetry is broken by quantum mechanical effect leading to dimensional transmutation i.e the quantum system, after renormalization, acquires an intrinsic length scale [3, 4]. Studies have been made on non-self-adjointness of the Hamiltonian in strongly attractive regime and how to do the self-adjoint extension of the same, which essentially amounts to renormalising the problem [5]. The system is also shown to exhibit limit cycle behaviour in renormalization group flow [6, 7]. Apart from being a place where sophisticated ideas of Quantum Field Theory gets realised, this potential appears in different branches of physics, starting from nuclear physics[7, 8], molecular physics [9] to quantum cosmology[10], study of black holes [11]. It deserves mentioning that the associated Schrodinger equation arises as a scalar wave equation for a field in Anti-de Sitter space-time. The second example that we are going to use to elucidate the idea is free particle.

The paper is organised in following manner. In section-II, we present the proof of our claim. In section-III, we review the quantum inverse square problem and we elucidate our claim using the same. In section-IV, we discuss the free particle case. In section-V, we generalise the theorem for any hermitian operator with definite scaling dimension. We conclude with a very brief discussion on the possible implication of the result obtained and its relation to anomaly in Conformal field theory.

S-THEOREM

To prove the theorem, we consider the eigenstates $|E\rangle$ of the Hamiltonian H and take expectation value of the

$[D, H]$ in these eigenstates. Now we have

$$\langle E|[D, H]|E\rangle = \langle E|DH|E\rangle - \langle E|HD|E\rangle \quad (0.3)$$

Assuming H is hermitian on a domain, which contains the state $D|E\rangle$, we have

$$\langle E|DH|E\rangle = E\langle E|D|E\rangle \quad (0.4)$$

$$\langle E|HD|E\rangle = E\langle E|D|E\rangle \quad (0.5)$$

Hence, using (0.4) and (0.5), (0.3) yields:

$$\langle E|[D, H]|E\rangle = 0 \quad (0.6)$$

It deserves mentioning that hermiticity of H is crucial in obtaining 0. Furthermore, we assumed H is hermitian on a domain that has $D|E\rangle$ states. We will elucidate how this assumptions are going to play a crucial role in subsequent sections. On the other hand, scale invariance implies

$$[D, H] = \nu zH, \quad (0.7)$$

so that we have

$$\langle E|[D, H]|E\rangle = \nu z\langle E|H|E\rangle \neq 0 \quad (0.8)$$

Comparing (0.6) and (0.8), we arrive at the incompatibility theorem. Note, the mismatch vanishes for $E = 0$ eigenstates. Hence, to apply the S-theorem, the existence of non-zero energy eigenstate is needed.

It deserves mentioning that the mismatch is not due to the real part of the quantity $\langle E|[D, H]|E\rangle$ since,

$$\text{Re}\langle E|[D, H]|E\rangle = 0 \quad (0.9)$$

is consistent with what we get using the algebra $[D, H] = \nu zH$ i.e

$$\text{Re}\langle E|[D, H]|E\rangle = \text{Re}\langle E|\nu zH|E\rangle = 0 \quad (0.10)$$

The mismatch between (0.6) and (0.8) lies in the imaginary part, which hints at the fact H can not be hermitian if we have scale invariance. We recall that hermiticity of H crucially depends on vanishing of a boundary term, which is imaginary when we consider quantities like $\langle E|H|E\rangle$.

ILLUSTRATION I: INVERSE SQUARE POTENTIAL

The aim of this section is to illustrate S-theorem with bound states. One of the examples where classically scale invariance is realised in a system is a particle moving in a inverse square potential. We consider a particle of mass

m moving in a inverse square potential. The action for the particle is given by

$$S = \int dt \left[\frac{1}{2} m \dot{r}^2 - \frac{\lambda'}{r^2} \right]. \quad (0.11)$$

where λ' is the coupling and $r > 0$ is the position of the particle.

We can redefine $r' \rightarrow \sqrt{m}r' = r$ and introduce a dimensionless coupling $\lambda = m\lambda'$ so that the action becomes

$$S = \int dt \frac{1}{2} \left[\dot{r}^2 - \frac{2\lambda}{r^2} \right] \quad (0.12)$$

The action (0.12) is indeed invariant under scale transformation, which acts on r in following manner:

$$r(t) \rightarrow s^{-\frac{1}{2}} r(st). \quad (0.13)$$

The Noether charge corresponding to this continuous scale symmetry is given by

$$D = \frac{rp}{2} + \frac{pr}{2} - tH \quad (0.14)$$

and scale invariance implies that D is conserved charge i.e $\frac{dD}{dt} = 0$.

Here we will briefly review the solution to the Schrodinger equation for inverse square potential [5]. The wave-function ψ obeys

$$-\frac{d^2\psi}{dr^2} + \frac{2\lambda}{r^2}\psi = E\psi \quad (0.15)$$

For the regime $2\lambda > -\frac{1}{4}$, the Hamiltonian is bounded below since we can rewrite $H = B^\dagger B$ where $B = -\frac{d}{dr} + \frac{\nu}{r}$ and $2\lambda = \nu^2 - \nu$, hence the energy eigenvalues are non-negative.

For the strongly attractive regime i.e $2\lambda < -\frac{1}{4}$, Hamiltonian is unbounded, we do have normalizable solution to (0.15) with negative E . The energy eigenstate with $E = -\kappa^2$ is given by

$$\psi = \kappa \sqrt{\frac{2 \sinh(\pi g)}{\pi g}} \sqrt{r} K_{ig}(\kappa r) \quad (0.16)$$

Just like what we did in the last section, we take energy eigenstates and calculate the expectation value of $[D, H]$ in those states. For strongly coupled regime, the inverse square potential admits bound states i.e states with negative energy ($-\epsilon_B$). Once again, there is a mismatch between calculation of this expectation value in

two different ways. First,

$$\begin{aligned}\langle E|[D, H]|E\rangle &= \langle E|DH|E\rangle - \langle E|HD|E\rangle \\ &= E\langle E|D|E\rangle - E\langle E|D|E\rangle = 0\end{aligned}\quad (0.17)$$

and secondly, we use the following commutator

$$[D, H] = 2iH \quad (0.18)$$

to arrive at

$$\langle E|[D, H]|E\rangle = 2i\langle E|H|E\rangle = -2i\epsilon_B \neq 0 \quad (0.19)$$

Naively, (0.17) and (0.19) seems to be incompatible. The resolution to this apparent contradiction illustrates the S-theorem. The fact that, in this regime, where we do have negative energy bound states, the Hamiltonian is no more a Hermitian operator, comes as a saviour and resolve the inconsistency in following way: in the second step of (0.17) when H is acting on bra $\langle E|$, we are implicitly assuming H is hermitian, which is not the case, hence (0.17) breaks down.

The following paragraph explains why and how H loses Hermiticity for strongly attractive regime i.e for $2\lambda < -\frac{1}{4}$.

To make sure, $H \supset p^2$ is a Hermitian operator, we must ensure the following term vanishes:

$$\left[\psi^* \frac{d\psi}{dr} - \psi \frac{d\psi^*}{dr} \right]_{r=0} = 0 \quad (0.20)$$

This ensures $\langle \psi|(H|\psi)\rangle = (\langle \psi|H)|\psi\rangle$. Physically this means that probability does not leak through the origin and the model is unitary. Now, any solution near $r = 0$ behaves as

$$\psi \sim r^{\Delta_+} + Ae^{i\theta}r^{\Delta_-} \quad (0.21)$$

where Δ_{\pm} are roots of $\Delta^2 - \Delta - 2\lambda = 0$.

$$\psi \sim r^{\frac{1}{2}+\nu} + Ae^{i\theta}r^{\frac{1}{2}-\nu} \quad (0.22)$$

where $\nu = \sqrt{-(2\lambda + \frac{1}{4})}$. Now it is easy to check, we can not enforce (0.20), if the solution is given by (0.22). It deserves mentioning that θ is not arbitrary, it can be obtained by doing a small r approximation of (0.16).

Similarly, to ensure

$$\langle \phi|(H|\psi)\rangle = (\langle \phi|H)|\psi\rangle, \quad (0.23)$$

we need

$$\left[\phi^* \frac{d\psi}{dr} - \psi \frac{d\phi^*}{dr} \right]_{r=0} = 0. \quad (0.24)$$

It can be shown for $\phi = \langle r|E\rangle$ and $\psi = \langle r|D|E\rangle$, (0.24) is not satisfied and if we consider the non-zero value

of $\left[\phi^* \frac{d\psi}{dr} - \psi \frac{d\phi^*}{dr} \right]_{r=0}$, we will see there is no mismatch between (0.17) and (0.19), since, (0.17) gets modified in that case so that H loses hermiticity.

In order to make H a Hermitian operator, we need to regularise and renormalise the problem which essentially introduces a scale and breaks the scale invariance. There is a plethora of literature on this regularisation and renormalization procedure in context of inverse square problem as mentioned in the introduction.

For the inverse square problem, the time translation generator H , the scale transformation generator $D' = \frac{D}{2}$ and special conformal generator $K = -2tD' + t^2H - \frac{r^2}{2}$ forms a close lie algebra known as $SO(2, 1)$ in following manner

$$\begin{aligned}[D', H] &= iH \\ [K, H] &= -2iD' \\ [D', K] &= -iK\end{aligned}$$

This algebra is the 0 + 1 dimensional version of conformal algebra, a symmetry algebra admitted by Conformal Field Theory (CFT) in d+1 dimension. This essentially means the Hamiltonian has a scaling dimension of 2. (In this convention, length has a scaling dimension of 1). In general, we could have a classically scale invariant system such that H has a scaling dimension z .

ILLUSTRATION II: FREE PARTICLE

In this section, we will illustrate S-theorem with scattering states. In principle, we can do this inverse square problem. But for simplicity, we take free particle ($H = \frac{p^2}{2}$), which also elucidates the scenario.

The fact that the scattering states $|p\rangle$ ($\langle x|p\rangle = e^{ipx}$) are dirac-delta normalized and hence, we have infinity all over our expressions (0.17) and (0.8) presents technical problem in showing there is a mismatch. To cure that, we put the theory on a circle with length L and at the end of the day, we take the decompactification limit i.e $L \rightarrow \infty$.

Since, we have scale invariance, S-theorem forbids H to be hermitian in this case. It motivates us to look carefully at the derivation of (0.6) and (0.17) in this context to check whether H is hermitian. In fact, it is not. It can be shown that although

$$\langle p|(HD|p)\rangle - (\langle p|DH)|p\rangle = 2ip^2L \quad (0.25)$$

is consistent with scaling algebra

$$[D, H] = 2iH \quad (0.26)$$

yet the cost of this consistency is that H is not hermitian on a domain which contains the state $D|p\rangle$ as evident from (0.25). Once again, the elegance of S-theorem is apparent. Now, we can decompactification limit, $2ip^2L$ becomes $2ip^2\delta(0)$, and we loose hermiticity of H in a same manner for the free particle on a line.

Given this scenario, we ask ourselves why we don't need to renormalise the problem to restore hermiticity of H . The answer is that we simply don't care; in case of a theory on a circle, the state $D|p\rangle$ does not belong to the Hilbert space since, $\langle x|D|p\rangle$ is not a periodic function living on a circle. Hence, it does not really matter if H looses hermiticity while acting on this kind of states. In the decompactification limit, this state does not enter the Hilbert space as well, since in $L \rightarrow \infty$, this state is not even dirac-delta normalized. Once again, it does not matter if H looses hermiticity on this space. As a comparison to inverse square problem, we note, there the state $D|E\rangle$ is properly normalized and we don't have the liberty of take this state out of Hilbert space, hence is the need of regularisation and renormalization and hence breaking of scale symmetry in quantum level. But here we have the liberty to take the state $D|p\rangle$ out of the Hilbert space so that S-theorem is not applicable and we are good.

GENERALISATION AND COROLLARY

S-theorem can be generalised to to any Hermitian operator A with non zero scaling dimension α i.e $[D, A] = i\alpha A$. Basically, H is replaced by the operator A , and the statement gets rephrased as A can not be Hermitian on a domain containing $D|A\rangle$ where $|A\rangle$ is the eigenstate of operator A . In particular, if we want A to hermitian on a Hilbert space, \mathcal{L}^2 space, then the state $D|A\rangle$ can not belong to the \mathcal{L}^2 space. For example, A can be the momentum operator p , which is hermitian on rigged Hilbert space and has a non-zero scaling dimension. Generalised S-theorem implies that $D|p\rangle$ can not belong to rigged Hilbert space, which is indeed the case.

A corollary of S-theorem is that we can not have bound states (i.e properly normalized) with non-zero energy in a scale invariant system if we want our Hamiltonian to be hermitian on Hilbert space. The proof goes in following way: If there exists a properly normalized state $|E\rangle$, then we expect $D|E\rangle$ to be a properly normalized state (which should be the case, since wavefunction dies out at infinity). In that case, we have a scale invariant

system, whose Hamiltonian H is Hermitian on a domain which contains $D|E\rangle$ states. Since, S-theorem forbids such situation, the only way it can happen is $\epsilon_B = 0$, for which, S-theorem is not applicable. Hence, bound state has to occur at $E = 0$ otherwise H becomes non-hermitian and the model becomes non-unitary, (for inverse square problem, this manifests itself as probability leaking through $r = 0$) if we retain the scale invariance. This result is in fact consistent with the representation theory: a discrete spectrum $\{E_n\}$ can not form a representation of a transformation which acts by $E \rightarrow \lambda^z E$ for continuous λ , implying that the only allowed values would be $E = 0, -\infty$, otherwise we have a continuous spectra and the system does not admit a ground state, in fact, we have shown for the inverse square problem that continuous spectrum is an illusion since in that case H is no more Hermitian.

CONCLUSION

In Conformal field theory trace anomaly indicates the breaking on scale invariance on quantum level i.e even at a fixed point trace of stress-energy tensor is non-zero. Now quantum mechanics can be thought of 0 + 1d field theory where $T_\mu^\mu = T_0^0 = H$, hence, In QM, expectation of H being non-zero can be thought of a signature of scale anomaly.

The theorem presented in this brief note does not really depend on number of dimension of the underlying theory. It is based on having a scaling algebra. Therefore, S-theorem holds even for field theories living in $d + 1$ dimension. It deserves mentioning that CFT in $d + 1 \geq 2$ involves radial quantization, where D becomes the generator of evolution operator. In that scenario, the scale invariance is maintained at the cost of loosing hermiticity of H , which does not play a significant role, since we are not doing time slice quantization. In time slice quantization, e^{iHt} is the evolution operator and we want it to be unitary and hence H should be hermitian. But in radial quantization e^{iHt} is not an evolution operator, hence, it is fine if H looses hermiticity.

To summarise, S-theorem is basically an incompatibility statement. Given a classically scale invariant physical system having non-zero energy eigenstates, we can

- break the scale invariance (e.g Inverse square strong coupling regime) or
- take the state $D|E\rangle$ out of Hilbert space (e.g free particle) or
- not worry about H being hermitian (for example CFT in $d + 1 \geq 2$)

What we want to do is dictated upon which kind of physics we are looking at and varies case to case. Moreover, the line of argument, presented here can be used to probe the normalizability of eigenstates of Hermitian operators with some scaling dimension and learn about the matrix elements of D between those eigenstates.

Last but not the least, S-theorem also explains why the quantum version of the virial theorem does not hold for inverse square potential. Classically, the virial theorem is valid for particles whose orbit is bounded in phase space, and it is a trivial task to show, that classically if there is bounded orbit, that has to be of 0 energy (since for a r^n potential $2\langle T \rangle = n\langle V \rangle$, where T and V are kinetic and potential energy of the system) and this is possible only if the spatial dimension is more than 1 and we can arrange for a situation where the angular momentum term cancel the original potential to make the effective potential vanish. This cancellation can occur only for inverse square potential since, the term due to angular momentum in effective potential is repulsive inverse square. But quantum mechanically, virial theorem seems to fail, since we do have bound states with finite non-zero binding energy for strongly attractive regime. The resolution to this apparent contradiction comes from noting that virial theorem does not apply to this case since it requires (0.17) to be valid, which is not the case as H is not Hermitian in strongly attractive regime. On the other hand, if we make H hermitian, we need to renormalise the problem and break the scale invariance, as a result, the potential is no more a homogeneous function of r , hence the virial theorem is not applicable.

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