PT SYMMETRY AS A NECESSARY AND SUFFICIENT CONDITION FOR UNITARY TIME EVOLUTION

HOW I UNDERSTAND BENDER'S BAG OF TRICKS

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1 Unitary time evolution for non-Hermitian Hamiltonians

$$i\frac{d}{dt}|R_i(t)\rangle = H|R_i(t)\rangle, \qquad -i\frac{d}{dt}\langle R_i(t)| = \langle R_i(t)|H^{\dagger}$$
(1)

$$\langle R_i(t)|e^{iH^{\dagger}t}e^{-iHt}|R_i(t)\rangle \neq \langle R_i(0)|R_i(0)\rangle.$$
(2)

Dirac norm not preserved in time if $H \neq H^{\dagger}$. Does not mean that theories cannot preserve norm if $U = e^{-iHt} \neq U^{\dagger}$. It only means cannot use Dirac norm. Since $i(d/dt)|R_i(t)\rangle = H|R_i(t)\rangle$ only involves ket, the choice of bra is not fixed. Thus there is freedom in choosing scalar product. So what is appropriate choice?

$$\langle R_j(t)|V|R_i(t)\rangle = e^{-i(E_i^R - E_j^R)t + (E_i^I + E_j^I)t} \langle R_j(t=0)|V|R_i(t=0)\rangle.$$
(3)

V-norm is time independent if

$$E_i^R - E_j^R = 0, \qquad E_i^I + E_j^I = 0, \quad \text{or } \langle R_j(t=0) | V | R_i(t=0) \rangle = 0.$$
 (4)

In general

$$i\frac{d}{dt}\langle R_j(t)|V|R_i(t)\rangle = \langle R_j(t)|(VH - H^{\dagger}V)|R_i(t)\rangle.$$
(5)

If states $|R_i(t)\rangle$ are complete, then necessary and sufficient condition for time independence is

$$VH - H^{\dagger}V = 0, \quad VHV^{-1} = H^{\dagger}.$$
 (6)

$$-i\frac{d}{dt}\langle R_i(t)|V = \langle R_i(t)|VH, \quad \langle L_i(t)| = \langle R_i(t)|V, \quad -i\frac{d}{dt}\langle L_i(t)| = \langle L_i(t)|H.$$
(7)

Thus general rule is to use overlap of left- and right-eigenvectors:

$$\langle L_i(t)|R_i(t)\rangle = \langle L_i(0)|R_i(0)\rangle \tag{8}$$

Generalize unitarity condition to (Mostafazadeh 2004):

$$U^{\dagger}(t) = e^{iH^{\dagger}t} = V e^{iHt} V^{-1} = V U^{-1}(t) V^{-1}.$$
(9)

With $\overrightarrow{H} = i\partial/\partial t$, $\overleftarrow{H} = -i\partial/\partial t$ (since [t, H] = -i), for wave functions have:

$$i\partial_t \left[\int dx \psi_i^{\mathrm{L}}(x,t) \psi_j^{\mathrm{R}}(x,t) \right] = \int dx \left[\psi_i^{\mathrm{L}}(x,t) \stackrel{\rightarrow}{H} \psi_j^{\mathrm{R}}(x,t) - \psi_i^{\mathrm{L}}(x,t) \stackrel{\leftarrow}{H} \psi_j^{\mathrm{R}}(x,t) \right].$$
(10)

If wave functions are well-behaved at infinity, then asymptotic surface term vanishes and V-norm is both time independent and finite. So normalize to

$$\int dx \psi_i^{\rm L}(x,t) \psi_j^{\rm R}(x,t) = \eta_i \delta_{i,j}.$$
(11)

However, in general V-norm need not be positive. So define up to $\eta_i = \pm 1$. Normalize phases to $\psi_j^{\mathrm{R}}(x,t) = \langle x | R_j(t) \rangle, \ \psi_i^{\mathrm{L}}(x,t) = \eta_i \langle L_i(t) | x \rangle$:

$$\int dx \psi_i^{\rm L}(x,t) \psi_j^{\rm R}(x,t) = \int dx \langle L_i(t) | x \rangle \eta_i \langle x | R_j(t) \rangle = \eta_i \langle L_i(t) | R_j(t) \rangle.$$
(12)

If we can introduce an operator C that obeys [C, H] = 0, $C^2 = I$, we can then identify $\eta_i = C_i$, and recognize V-norm as

$$\int dx \psi_i^{\rm L}(x,t) C_i \psi_j^{\rm R}(x,t) = \langle L_i(t) | R_j(t) \rangle = \langle R_i(t) | V | R_j(t) \rangle,$$
(13)

viz. precisely the C-norm of PT theories. Moreover, if energy spectrum is both real and complete, we can bring H to a Hermitian form \tilde{H} by a similarity transformation, with $\langle L_i(t)|R_j(t)\rangle$ then being positive, just as required of a probability. If on the other hand some of the energy eigenvalues of H appear in complex pairs, then V-norm is now a transition matrix element and need not be positive. Also, eigenstates of H do not have to be complete.

2 PT symmetry and the $VHV^{-1} = H^{\dagger}$ condition

If $VHV^{-1} = H^{\dagger}$, then H and H^{\dagger} have same energy eigenvalues, and those eigenvalues are either real or appear in complex conjugate pairs.

If eigenvalues of H are either real or appear in complex conjugate pairs, then H and H^{\dagger} have same energy eigenvalues, and there must thus exist a V that effects $VHV^{-1} = H^{\dagger}$.

If $f(\lambda) = |H - \lambda I|$ is a real function of λ , then eigenvalues of H are real or appear in complex conjugate pairs. If eigenvalues of H are either real or appear in complex conjugate pairs, then $f(\lambda)$ is a real function of λ . Bender, Berry and Mandilara (2002): If [H, PT] = 0, then $f(\lambda) = |H - \lambda I|$ is a real function of λ . Bender and Mannheim (2010): If $f(\lambda) = |H - \lambda I|$ is a real function of λ , then [H, PT] = 0.

PT symmetry is equivalent to $VHV^{-1} = H^{\dagger}$, and thus PT symmetry is both necessary and sufficient for unitary time evolution. Thus even if cannot construct V explicitly, which is usually the case, can test for unitarity by use of a symmetry alone. PT symmetry is thus the general diagnostic for unitarity.

Bender and Mannheim (2010): If [H, PT] = 0 and energy eigenspectrum of H is complete, then C operator that obeys [C, H] = 0, $C^2 = I$ necessarily exists.

Three cases of interest when [H, PT] = 0:

(1) Eigenvalues of H real and complete.

(2) Eigenvalues of H complete but include one or more complex conjugate pairs.

(3) Eigenvalues of H are incomplete (Jordan-block, exceptional point case).

Bender and Mannheim (2010): If (1), then [C, PT] = 0. If (2), then $[C, PT] \neq 0$. If (3), then C does not exist.

3 Unitarity when energies are all real and complete

$$BHB^{-1} = \hat{H} = \hat{H}^{\dagger} \tag{14}$$

$$B^{\dagger}BHB^{-1}(B^{\dagger})^{-1} = H^{\dagger}.$$
 (15)

Identify $V = B^{\dagger}B$. V is a positive operator (often written $V = e^{-Q}$), so set $V = B^{\dagger}B = G^2$. G also a positive operator that obeys $G = G^{\dagger}$ and yields a Hamiltonian $\tilde{H} = GHG^{-1}$ that is Hermitian (Mostafazadeh 2002). Obtain $(GB^{-1})^{\dagger} = BG^{-2}G = BG^{-1} = (GB^{-1})^{-1}$. Thus GB^{-1} is unitary, as it must be.

Choice of V not unique. Can set $B^{\dagger}BCHCB^{-1}(B^{\dagger})^{-1} = H^{\dagger}$ and thus use $V' = VC = B^{\dagger}BC$. If can set V = PC then V' = VC = P and $PHP = H^{\dagger}$. The utility of this choice is that if we continue to an exceptional point, then C, V and G all become singular and undefined (cannot diagonalize a non-diagonalizable Hamiltonian), but can still relate H and H^{\dagger} (since $|H - \lambda I|$ remains real in the limit). Thus must be able to relate H and H^{\dagger} by a non-singular operator that is continuous in the limit. Hence P. Thus V' is non-singular in the limit, even though V is singular.

Set
$$H|n_i\rangle = E_i|n_i\rangle$$
, $\tilde{H}|\tilde{n}_i\rangle = E_i|\tilde{n}_i\rangle = E_iGHG^{-1}|\tilde{n}_i\rangle$.
 $|\tilde{n}_i\rangle = G|n_i\rangle$, $\langle \tilde{n}_i| = \langle n_i|G^{\dagger} = \langle n_i|G$.
 $\langle n_j|V|n_i\rangle = \langle n_j|G^2|n_i\rangle = \langle \tilde{n}_j|\tilde{n}_i\rangle = \delta_{i,j}$.
 $I = \sum_i |\tilde{n}_i\rangle \langle \tilde{n}_i| = \sum_i G|n_i\rangle \langle n_i|G$.
 $\sum_i |n_i\rangle \langle n_i|G^2 = \sum_i |n_i\rangle \langle n_i|V = I$.

G effects transformation from a skew basis $|n_i\rangle$ to an orthogonal basis $|\tilde{n}_i\rangle$, and thus cannot be unitary. Since H is a Hermitian Hamiltonian \tilde{H} in disguise when all energies are real, it must be unitary in disguise too.

In \tilde{H} basis set $\tilde{S} = \sum_i |\tilde{n}_{in}\rangle \langle \tilde{n}_{out}|$. Then $\tilde{S}\tilde{S}^{\dagger} = I$. In H basis define $S = \sum_i |n_{in}\rangle \langle n_{out}|G^2$. Then by mapping we have $\tilde{S} = GSG^{-1}$, and thus

$$SG^{-2}S^{\dagger}G^{2} = I, \qquad G^{2}SG^{-2}S^{\dagger} = I, \qquad SV^{-1}S^{\dagger}V = I, \qquad VSV^{-1}S^{\dagger} = I.$$
 (16)

This is the unitarity relation when energies are all real and eigenvectors are complete.

Can also derive directly in V-norm basis where

$$\langle n_{in}^{i} | V | n_{in}^{j} \rangle = \langle n_{in}^{j} | V^{\dagger} | n_{in}^{i} \rangle = \delta_{i,j}, \qquad \langle n_{out}^{i} | V | n_{out}^{j} \rangle = \langle n_{out}^{j} | V^{\dagger} | n_{out}^{i} \rangle = \delta_{i,j},$$

$$\sum_{i} | n_{in}^{i} \rangle \langle n_{in}^{i} | V = \sum_{i} V^{\dagger} | n_{in}^{i} \rangle \langle n_{in}^{i} | = I, \qquad \sum_{i} | n_{out}^{i} \rangle \langle n_{out}^{i} | V = \sum_{i} V^{\dagger} | n_{out}^{i} \rangle \langle n_{out}^{i} | = I.$$

$$(17)$$

Now define $S = \sum_{i} |n_{in}\rangle \langle n_{out}|V$, to obtain

$$SV^{-1}S^{\dagger}V = \sum_{i} |n_{in}^{i}\rangle \langle n_{out}^{i}|VV^{-1}\sum_{j}V^{\dagger}|n_{out}^{j}\rangle \langle n_{in}^{j}|V = \sum_{i} |n_{in}^{i}\rangle \langle n_{in}^{i}|V = I.$$
(18)

$$SV^{-1}S^{\dagger}V = I, \qquad VSV^{-1}S^{\dagger} = I.$$
⁽¹⁹⁾

Since no reference to \tilde{H} , now holds even if energies are not all real (but still complete). Utility is that even if cannot prepare unstable in states, still need them for completeness, and thus can generate unstable out states in a unitarity preserving manner, even if have modes that grow in time.

Bender and Mannheim (2008): When energy eigenvectors not complete, find that instead solutions to timedependent Schrödinger equation are complete. Then can construct wave packets out of them that preserve norms of wave packets in time.

3.1 A simple example

$$H = r\cos\theta\sigma_0 + ir\sin\theta\sigma_3 + s\sigma_1 = \begin{pmatrix} r\cos\theta + ir\sin\theta & s\\ s & r\cos\theta - ir\sin\theta \end{pmatrix}.$$
 (20)

H is *PT* symmetric under $P = \sigma_1$, T = K. $PHP = H^{\dagger}$. Energies $E_{\pm} = r \cos \theta \pm (s^2 - r^2 \sin \theta^2)^{1/2}$. If $s^2 - r^2 \sin \theta^2$ is positive, energies are real. Define $\sin \alpha = (s^2 - r^2 \sin \theta^2)^{1/2}/s$, $\cos \alpha = r \sin \theta/s$.

$$G^{\pm 1} = \left(\frac{1+\sin\alpha}{2\sin\alpha}\right)^{1/2} \sigma_0 \pm \sigma_2 \left(\frac{1-\sin\alpha}{2\sin\alpha}\right)^{1/2}, \qquad G^{\pm 2} = V^{\pm 1} = \frac{1}{\sin\alpha} \sigma_0 \pm \sigma_2 \frac{\cos\alpha}{\sin\alpha}, \tag{21}$$

$$VHV^{-1} = H^{\dagger}, \qquad \tilde{H} = GHG^{-1} = r\cos\theta\sigma_0 + \sigma_1(s^2 - r^2\sin^2\theta)^{1/2}.$$
 (22)

Eigenvalues of G are $[(1 \pm \sin \alpha)/2 \sin \alpha)]^{1/2}$. Eigenvalues of $G^2 = V$ are $(1 \pm \cos \alpha)/\sin \alpha$. All eigenvalues are real and positive.

$$C = \frac{1}{\sin \alpha} \left(\sigma_1 + i \cos \alpha \sigma_3 \right), \qquad [C, PT] = 0.$$
(23)

$$u_{+} = \frac{e^{-i(r\cos\theta + \mu)t}e^{i\pi/4}}{(2\sin\alpha)^{1/2}} \begin{pmatrix} e^{-i\alpha/2} \\ -ie^{i\alpha/2} \end{pmatrix}, \qquad u_{-} = \frac{e^{-i(r\cos\theta - \mu)t}e^{i\pi/4}}{(2\sin\alpha)^{1/2}} \begin{pmatrix} ie^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix}, \qquad \mu = (s^{2} - r^{2}\sin\theta^{2})^{1/2}.$$
(24)

$$u_{\pm}^{\dagger}Vu_{\pm} = +1, \qquad u_{\pm}^{\dagger}Vu_{\mp} = 0, \qquad u_{+}u_{+}^{\dagger}V + u_{-}u_{-}^{\dagger}V = I.$$
 (25)

Basis is V-othornormal. All of V, G, and C become undefined at $\alpha = 0$, the exceptional point at which E_+ and E_- become equal, u_+ and u_- become equal, and H becomes a non-diagonalizable Jordan-block Hamiltonian. However at this point P is still non-singular and $PHP = H^{\dagger}$ still holds.

4 Unitarity when energies are not all real but complete

Define
$$\nu = (r^2 \sin \theta^2 - s^2)^{1/2}$$
, $E_{\pm} = r \cos \theta \pm i\nu$, $\sinh \beta = (r^2 \sin \theta^2 - s^2)^{1/2}/s$, $\cosh \beta = r \sin \theta/s$

$$G^{\pm 1} = \left(\frac{1+i\sinh\beta}{2i\sinh\beta}\right)^{1/2} \sigma_0 \pm \sigma_2 \left(\frac{1-i\sinh\beta}{2i\sinh\beta}\right)^{1/2} \neq (G^{\pm 1})^{\dagger}, \quad G^{\pm 2} = V^{\pm 1} = \frac{1}{i\sinh\beta} \sigma_0 \pm \sigma_2 \frac{\cosh\beta}{i\sinh\beta}. \tag{26}$$

 $G \neq G^{\dagger}, \quad V \neq V^{\dagger}, \quad VHV^{-1} = H^{\dagger}, \qquad \tilde{H} = GHG^{-1} = r\cos\theta\sigma_0 + i\sigma_1(r^2\sin^2\theta - s^2)^{1/2} \neq \tilde{H}^{\dagger}.$ (27)

$$C = V^{-1}P = \frac{1}{i\sinh\beta} \left(\sigma_1 + i\cosh\beta\sigma_3\right), \qquad [C, PT] \neq 0.$$
(28)

$$u_{+} = \frac{e^{-ir\cos\theta t + \nu t}}{(2\sinh\beta)^{1/2}} \begin{pmatrix} e^{\beta/2} \\ -ie^{-\beta/2} \end{pmatrix}, \quad u_{-} = \frac{e^{-ir\cos\theta t - \nu t}}{(2\sinh\beta)^{1/2}} \begin{pmatrix} ie^{-\beta/2} \\ e^{\beta/2} \end{pmatrix}.$$
(29)

$$u_{\pm}^{\dagger}Vu_{\pm} = 0, \qquad u_{-}^{\dagger}Vu_{+} = +1, \qquad u_{+}^{\dagger}Vu_{-} = -1, \qquad u_{+}u_{-}^{\dagger}V - u_{-}u_{+}^{\dagger}V = I.$$
 (30)

$$D(E) = \frac{u_{-}^{\dagger} V u_{+}}{E - (E_R - iE_I)} + \frac{u_{+}^{\dagger} V u_{-}}{E - (E_R + iE_I)},$$
(31)

$$D(E) = \frac{1}{E - (E_R - iE_I)} - \frac{1}{E - (E_R + iE_I)} = \frac{-2iE_I}{(E - E_R)^2 + E_I^2}.$$
(32)

Imaginary part has same sign as standard Breit-Wigner, where one assumes Im(E) < 0, to thus justify its use:

$$D_{\rm BW}(E) = \frac{1}{E - (E_R - iE_I)} = \frac{E - E_R - iE_I}{(E - E_R)^2 + E_I^2}.$$
(33)

Thus role of minus sign in $u_{+}^{\dagger}Vu_{-} = -1$ is to restore unitarity, not violate it. Compare with Lee-Wick.

5 Unitarity when energies are all real but incomplete

$$M = \begin{pmatrix} a & 1\\ 0 & a \end{pmatrix}. \tag{34}$$

$$\begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad a \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix}.$$
(35)

6 Constructing the non-diagonalizable case as a limit of a diagonalizable one

$$\sigma_1 H \sigma_1 = \sigma_1 (r \cos \theta \sigma_0 + ir \sin \theta \sigma_3 + s\sigma_1) \sigma_1 = r \cos \theta \sigma_0 - ir \sin \theta \sigma_3 + s\sigma_1 = H^{\dagger}, \qquad (36)$$

$$B^{\dagger}BCHCB^{-1}(B^{\dagger})^{-1} = H^{\dagger}, \tag{37}$$

$$V' = VC = P, (38)$$

$$PHP = H^{\dagger}.$$
(39)

7 Symplectic symmetry and Stokes wedges in classical mechanics

$$\{u, v\} = \sum_{i} \left(\frac{\partial u}{\partial q_{i}} \frac{\partial v}{\partial p_{i}} - \frac{\partial u}{\partial p_{i}} \frac{\partial v}{\partial q_{i}} \right).$$

$$(40)$$

$$\eta = \begin{pmatrix} q_i \\ p_i \end{pmatrix} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \text{ If use } (q_1, p_1, q_2, -p_2), \text{ then } J = C = \begin{pmatrix} -i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix}, \quad C\gamma_{\mu}C^{-1} = -\widetilde{\gamma_{\mu}}.$$
(41)

$$\{u, v\} = \frac{\partial \widetilde{u}}{\partial \eta} J \frac{\partial v}{\partial \eta}.$$
(42)

$$M_{ij} = \frac{\partial \xi_i}{\partial \eta_j}, \qquad \frac{\partial v}{\partial \eta} = \tilde{M} \frac{\partial v}{\partial \xi}, \qquad \frac{\partial \tilde{u}}{\partial \eta} = \frac{\partial \tilde{u}}{\partial \xi} M.$$
(43)

$$\{u,v\} = \frac{\partial \widetilde{u}}{\partial \xi} M J \widetilde{M} \frac{\partial v}{\partial \xi}.$$
(44)

$$\{u, v\} = \frac{\partial \tilde{u}}{\partial \xi} J \frac{\partial v}{\partial \xi} \quad \text{if} \quad M J \tilde{M} = J, \quad \text{symplectic symmetry.}$$
(45)

$$M = e^{i\omega_i G_i}, \quad e^{i\omega_i G_i} J e^{i\omega_i \tilde{G}_i} = J, \quad G_i J + J \tilde{G}_i = 0, \quad \tilde{G}_i = -J^{-1} G_i J = J G_i J.$$

$$(46)$$

solve via
$$G_i J - JG_i = 0$$
 and $G_i = -G_i$, or $G_i J + JG_i = 0$ and $G_i = G_i$. (47)

In N dimensions have N antisymmetric and N(N-1)/2 symmetric generators. Algebra closes on Sp(N) with N(N+1)/2 generators. In classical mechanics can make all G_i be pure imaginary, so that with real ω_i all M are real. However, invariance under canonical transformations persists if ω_i are complex. Continuing to complex ω_i only has content if we encounter a Stokes line in a complex q_i, p_i phase space. In each Stokes wedge we can construct a canonical quantization (Poisson brackets become commutators) with an associated correspondence principle (classical coordinates are eigenvalues of quantum operators).

8 Comparing *PT* symmetry and Hermiticity

- 1. Hermiticity is sufficient to yield real energy eigenvalues, but not necessary. PT symmetry is necessary to produce real eigenvalues but not sufficient. [H, PT] = 0 and [C, PT] = 0 combined is both necessary and sufficient to yield real eigenvalues. PT symmetry is necessary and sufficient to yield a real $f(\lambda) = |H \lambda I|$.
- 2. Hermiticity is sufficient to yield unitary time evolution, but not necessary. PT symmetry is both necessary and sufficient to yield unitary time evolution.
- 3. Hermiticity cannot describe unstable states or non-diagonalizable Hamiltonians. PT symmetry can describe both unstable states (loss-gain systems) and non-diagonalizable Hamiltonians (conformal gravity).
- 4. [PT, H] = 0 commutator is preserved by a similarity transformation. The relation $H_{ij} = H_{ji}^*$ is **basis** dependent and not preserved by a similarity transformation. If $H = H^{\dagger}$ and $H' = SHS^{-1}$, then $H'^{\dagger} = S^{-1\dagger}H^{\dagger}S^{\dagger} = S^{-1\dagger}HS^{\dagger} = S^{-1\dagger}S^{-1}H'SS^{\dagger} = (SS^{\dagger})^{-1}H'SS^{\dagger}$. If $S^{\dagger} \neq S^{-1}$, $H'^{\dagger} \neq H'$.
- 5. General basis-independent definition of Hermitian: eigenvalues are real and eigenstates are complete. General basis-independent definition of PT symmetry: secular determinant $f(\lambda) = |H - \lambda I|$ is real.
- 6. Bender (2007): PT is physical. Hermiticity is mathematical.
- 7. Bender and Mannheim (2011): PT has a natural connection to Lorentz invariance: $P\bar{x}P = -\bar{x}, TtT = -t, PTx_{\mu}TP = -x_{\mu}$ (equivalent to Lorentz boost though complex $i\pi$).
- 8. For a Hermitian operator Dirac norm can be assigned a priori. It is dynamics independent, and is just like a flat space Euclidean or Minkowski metric $ds^2 = \eta_{\mu\nu} dx^{\mu} dx^{\nu}$. For the *PT* case, the V-norm cannot be preassigned. It is dynamics dependent, and is just like general relativity line element $ds^2 = g_{\mu\nu}(x) dx^{\mu} dx^{\nu}$, where $g_{\mu\nu}(x)$ is determined by gravitational equations of motion.

- 9. *PT* can be defined at the c-number level. Hermiticity can only be defined as a q-number property of the quantum Hilbert space.
- 10. PT can be defined as a symmetry on both stationary and non-stationary paths in the Feynman path integral $\int D[x]e^{iS_{\text{CL}}(x,x')}$. No reference is made to Hermiticity or Hilbert space in path integral, a purely classical c-number approach to quantization, and no notion of Hermiticity can be attached to any of the classical paths, be they stationary or non-stationary.
- 11. Thus where does Hermiticity come from, and how did it come into physics? And how can we tell from a c-number path integral whether or not the associated q-number theory is Hermitian, PT, or neither? I.e. knowing only the c-number propagator G(x', t'; x, t), how do we determine what quantum matrix element it is to represent, $\langle \Omega_{\rm R} | T(\phi(x)\phi(x') | \Omega_{\rm R} \rangle$, or $\langle \Omega_{\rm L} | T(\phi(x)\phi(x') | \Omega_{\rm R} \rangle = \langle \Omega_{\rm R} | VT(\phi(x)\phi(x') | \Omega_{\rm R} \rangle$, or something else?

8.1 *PT* symmetry and path integration

Define $\theta(t'-t)\psi(x',t') = i\int dx G(x',t';x,t)\psi(x,t)$. If $i\partial_t\psi(x,t) = H(x,t)\psi(x,t)$, then propagator obeys

$$[i\partial_{t'} - H(x', -i\partial_{x'}, t')]G(x', t'; x, t) = \delta(x - x')\delta(t - t').$$
(48)

If H is Hermitian, three ways to represent the propagator:

- (1) *H* is generator of time translations: $G(x', t'; x, t) = -i\theta(t' t)\langle x, t | x', t' \rangle = -i\theta(t' t)\langle x | e^{-iH(t'-t)} | x' \rangle$. (2) Completeness of energy eigenfunctions: $G(x', t'; x, t) = -i\theta(t' - t)\sum_{i} u_i^*(x')u_i(x)e^{-iE_i(t'-t)}$.
- (3) Completeness of eigenstates of \hat{x} and \hat{p} operators that obey $[\hat{x}, \hat{p}] = i$ to get Feynman path integral:

$$G(x', t + \epsilon; x, t) = -i\theta(\epsilon) \langle x | \left[1 - i\epsilon \frac{\hat{p}^2}{2m} - i\epsilon V(\hat{x}) \right] | x' \rangle$$

$$= -i\theta(\epsilon) \left[\delta(x' - x) [1 - i\epsilon \bar{V}(x, x')] - i\epsilon \int \frac{dp}{2\pi} \frac{p^2}{2m} e^{ip(x' - x)} \right]$$

$$= -i\theta(\epsilon) \int \frac{dp}{2\pi} e^{ip(x' - x)} \left[1 - i\epsilon \frac{p^2}{2m} - i\epsilon \bar{V}(x'x) \right]$$

$$= -i\theta(\epsilon) \int \frac{dp}{2\pi} \exp \left[ip(x' - x) - i\epsilon \frac{p^2}{2m} - i\epsilon \bar{V}(x'x) \right]$$

$$= -i\theta(\epsilon) \left(\frac{m}{2\pi i\epsilon} \right)^{1/2} \exp \left[\frac{im(x' - x)^2}{2\epsilon} - i\epsilon \bar{V}(x'x) \right].$$
(49)

$$G(x', t + \epsilon; x, t) = -i\theta(\epsilon) \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} e^{iS_{\rm CL}(x', x)}.$$
(50)

If H is not Hermitian but PT symmetric:

(1) is same.

(2) is replaced by $G(x', t'; x, t) = -i\theta(t'-t)\sum_i \psi_i^{\mathrm{R}}(x)C_i\psi_i^{\mathrm{L}}(x)e^{-iE_i(t'-t)}$.

(3) still uses completeness of momentum and position eigenstates, except realize $[\hat{x}, \hat{p}] = i$ as $[e^{i\theta}x, -ie^{-i\theta}\partial_x] = i$ in appropriate Stokes wedge in complex coordinate plane.

If start with c-number path integral representation $G(x', t'; x, t) = -i\theta(t'-t)\int D[x]e^{iS_{CL}(x,x')}$, then

(1) If path integral exists with real measure, quantum H is Hermitian.

(2) If path integral only exists with complex measure, quantum H is not Hermitian.

(3) If path integral only exists with complex measure, and Euclidean time continuation is real, quantum H is PT symmetric.

8.2 *PT* symmetry and the Pais-Uhlenbeck fourth-order oscillator

$$I_{\rm PU} = \frac{\gamma}{2} \int dt \left[\ddot{z}^2 - \left(\omega_1^2 + \omega_2^2\right) \dot{z}^2 + \omega_1^2 \omega_2^2 z^2 \right], \qquad \frac{d^4 z}{dt^4} + (\omega_1^2 + \omega_2^2) \frac{d^2 z}{dt^2} + \omega_1^2 \omega_2^2 z = 0.$$
(51)

$$x = \dot{z}, \quad H_{\rm PU} = \frac{p_x^2}{2\gamma} + p_z x + \frac{\gamma}{2} \left(\omega_1^2 + \omega_2^2\right) x^2 - \frac{\gamma}{2} \omega_1^2 \omega_2^2 z^2, \qquad G(E) = \frac{1}{\omega_1^2 - \omega_2^2} \left(\frac{1}{E^2 - \omega_1^2} - \frac{1}{E^2 - \omega_2^2}\right). \tag{52}$$

$$\omega_{i} = (\bar{k}^{2} + M_{i}^{2})^{1/2}, \quad I_{\rm S} = -\frac{1}{2} \int d^{4}x \left[\partial_{\mu} \partial_{\nu} \phi \partial^{\mu} \partial^{\nu} \phi + (M_{1}^{2} + M_{2}^{2}) \partial_{\mu} \phi \partial^{\mu} \phi + M_{1}^{2} M_{2}^{2} \phi^{2} \right], \tag{53}$$

$$(-\partial_t^2 + \bar{\nabla}^2 - M_1^2)(-\partial_t^2 + \bar{\nabla}^2 - M_2^2)\phi(x) = 0,$$
(54)

$$D(k, M_1, M_2) = \frac{1}{(M_2^2 - M_1^2)} \left(\frac{1}{k^2 + M_1^2} - \frac{1}{k^2 + M_2^2} \right),$$
(55)

$$T_{00}(M_1, M_2) = \pi_0 \dot{\phi} + \frac{1}{2} \left[\pi_{00}^2 + (M_1^2 + M_2^2) (\dot{\phi}^2 - \partial_i \phi \partial^i \phi) - M_1^2 M_2^2 \phi^2 - \pi_{ij} \pi^{ij} \right],$$
(56)

$$\pi^{\mu} = \frac{\partial L}{\partial \phi_{,\mu}} - \partial_{\lambda} \left(\frac{\partial L}{\partial \phi_{,\mu,\lambda}} \right) = -(M_1^2 + M_2^2) \partial^{\mu} \phi + \partial_{\lambda} \partial^{\mu} \partial^{\lambda} \phi, \quad \pi^{\mu\lambda} = \frac{\partial L}{\partial \phi_{,\mu,\lambda}} = -\partial^{\mu} \partial^{\lambda} \phi,$$

$$[\phi(\bar{x}, t), \pi_0(\bar{x}', t)] = i\hbar \delta^3(\bar{x} - \bar{x}'), \quad [\partial_0 \phi(\bar{x}, t), \pi^0_0(\bar{x}', t)] = i\hbar \delta^3(\bar{x} - \bar{x}'). \tag{57}$$

Second-order Klein-Gordon wave equation has both positive and negative frequency solutions. But Hamiltonian is positive definite, so no transitions to negative frequency. Fourth-order wave equation also has both positive and negative frequency solutions. If Hamiltonian is Hermitian, Hamiltonian is unbounded from below. However, if Hamiltonian is PT symmetric and ϕ or z is anti-Hermitian, Hamiltonian then is bounded from below, and there are no transitions to negative frequency. Also no states of negative norm (Bender and Mannheim 2008).

A Distinguishing \hat{H} and \tilde{H} and the lack of uniqueness of V

$$\hat{H} = a_0 \sigma_0 + a_1 \sigma_1 + a_2 \sigma_2 + a_3 \sigma_3, \tag{A1}$$

$$B = \frac{1}{i\sqrt{3}}(\sigma_0 + 2\sigma_1), \quad B^{-1} = \frac{1}{i\sqrt{3}}(\sigma_0 - 2\sigma_1).$$
(A2)

$$H = a_0 \sigma_0 + a_1 \sigma_1 - \frac{\sigma_2}{3} (5a_2 + 4ia_3) - \frac{\sigma_3}{3} (5a_3 - 4ia_2).$$
(A3)

$$V = \frac{1}{3}(5+4\sigma_1), \quad V^{-1} = \frac{1}{3}(5-4\sigma_1), \tag{A4}$$

$$VHV^{-1} = a_0\sigma_0 + a_1\sigma_1 - \frac{\sigma_2}{3}(5a_2 - 4ia_3) - \frac{\sigma_3}{3}(5a_3 + 4ia_2),$$
(A5)

$$G = \frac{1}{\sqrt{3}}(2\sigma_0 + \sigma_1), \quad G^{-1} = \frac{1}{\sqrt{3}}(2\sigma_0 - \sigma_1)$$
(A6)

$$GHG^{-1} = \tilde{H} = a_0\sigma_0 + a_1\sigma_1 - a_2\sigma_2 - a_3\sigma_3, \tag{A7}$$

$$BG^{-1}\tilde{H}GB^{-1} = \hat{H} \tag{A8}$$

is unitary, just as required.

$$H = h_0 \sigma_0 + \boldsymbol{\sigma} \cdot \mathbf{h} \tag{A9}$$

$$P = \frac{\boldsymbol{\sigma} \cdot \mathbf{h}_{\mathrm{R}}}{(\mathbf{h}_{\mathrm{R}} \cdot \mathbf{h}_{\mathrm{R}})^{1/2}}, \quad T = K \frac{\sigma_2 \boldsymbol{\sigma} \cdot \mathbf{h}_{\mathrm{R}} \times \mathbf{h}_{\mathrm{I}}}{(\mathbf{h}_{\mathrm{R}} \times \mathbf{h}_{\mathrm{I}} \cdot \mathbf{h}_{\mathrm{R}} \times \mathbf{h}_{\mathrm{I}})^{1/2}}, \quad C = \frac{\boldsymbol{\sigma} \cdot \mathbf{h}}{(\mathbf{h} \cdot \mathbf{h})^{1/2}}, \quad (A10)$$

$$PHP = H^{\dagger}, \quad PCHCP = H^{\dagger}.$$
 (A11)

$$PC = \frac{(\mathbf{h}_{\mathrm{R}} \cdot \mathbf{h}_{\mathrm{R}} - \boldsymbol{\sigma} \cdot \mathbf{h}_{\mathrm{R}} \times \mathbf{h}_{\mathrm{I}})}{(\mathbf{h}_{\mathrm{R}} \cdot \mathbf{h}_{\mathrm{R}})^{1/2} (\mathbf{h} \cdot \mathbf{h})^{1/2}}.$$
(A12)

$$\operatorname{Tr}[PC] = \frac{2\mathbf{h}_{\mathrm{R}} \cdot \mathbf{h}_{\mathrm{R}}}{(\mathbf{h}_{\mathrm{R}} \cdot \mathbf{h}_{\mathrm{R}})^{1/2}(\mathbf{h} \cdot \mathbf{h})^{1/2}}, \quad \operatorname{Det}[PC] = I,$$
(A13)

$$\mathbf{h}_{\mathrm{R}} = \left(a_{1}, -\frac{5a_{2}}{3}, -\frac{5a_{3}}{3}\right), \quad \mathbf{h}_{\mathrm{I}} = \left(0, -\frac{4a_{3}}{3}, \frac{4a_{2}}{3}\right), \tag{A14}$$

$$PV = \frac{1}{3(\mathbf{h}_{\mathrm{R}} \cdot \mathbf{h}_{\mathrm{R}})^{1/2}} (4h_{1}^{\mathrm{R}} + 5\boldsymbol{\sigma} \cdot \mathbf{h}), \qquad (A15)$$

$$a = -\frac{5b\mathbf{h} \cdot \mathbf{h}}{4h_1^{\rm R}} = -\frac{5b(a_1^2 + a_2^2 + a_3^2)}{4a_1},$$

$$b = \frac{12h_1^{\rm R}(\mathbf{h}_{\rm R} \cdot \mathbf{h}_{\rm R})^{1/2}}{[16(h_1^{\rm R})^2 - 25\mathbf{h} \cdot \mathbf{h}](\mathbf{h} \cdot \mathbf{h})^{1/2}} = -\frac{4a_1}{[9a_1^2 + 25(a_2^2 + a_3^2)]^{1/2}(a_1^2 + a_2^2 + a_3^2)^{1/2}},$$
(A16)