Biorthogonal Quantum Mechanics
— an overview —

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Eigenstates of complex Hamiltonians and their adjoints

We begin by reviewing properties of eigenstates of generic complex Hamiltonians in finite dimensions.

Let $\hat{K} = \hat{H} - \mathrm{i}\hat{\Gamma}$, with $\hat{H}^\dagger = \hat{H}$ and $\hat{\Gamma}^\dagger = \hat{\Gamma}$, be a complex Hamiltonian with eigenstates $\{|\phi_n\rangle\}$ and eigenvalues $\{\kappa_n\}$:

$$\hat{K}|\phi_n\rangle = \kappa_n|\phi_n\rangle \quad \text{and} \quad \langle\phi_n|\hat{K}^\dagger = \bar{\kappa}_n\langle\phi_n|. \tag{1}$$

We assume for now that the eigenvalues $\{\kappa_n\}$ are not degenerate.

It will be convenient to introduce eigenstates of the Hermitian adjoint matrix $\hat{K}^\dagger$:

$$\hat{K}^\dagger|\chi_n\rangle = \nu_n|\chi_n\rangle \quad \text{and} \quad \langle\chi_n|\hat{K} = \bar{\nu}_n\langle\chi_n|. \tag{2}$$

Here and in what follows, a 'Hermitian adjoint' will be defined by the convention that $\hat{K}^\dagger$ denotes the complex-conjugate transpose of $\hat{K}$.

The reason for introducing the additional states $\{|\chi_n\rangle\}$ is because the eigenstates $\{|\phi_n\rangle\}$ of $\hat{K}$ are in general not orthogonal:

$$\langle\phi_m|\phi_n\rangle = 2\mathrm{i}\frac{\langle\phi_m|\hat{\Gamma}|\phi_n\rangle}{\bar{\kappa}_m - \kappa_n} = 2\frac{\langle\phi_m|\hat{H}|\phi_n\rangle}{\bar{\kappa}_m + \kappa_n} \tag{3}$$

for $m \neq n$, which follows from $2\mathrm{i}\hat{\Gamma} = \hat{K}^\dagger - \hat{K}$ and that $2\hat{H} = \hat{K}^\dagger + \hat{K}$.

An analogous result

$$\langle\chi_m|\chi_n\rangle = 2\mathrm{i}\frac{\langle\chi_m|\hat{\Gamma}|\chi_n\rangle}{\nu_n - \bar{\nu}_m} = 2\frac{\langle\chi_m|\hat{H}|\chi_n\rangle}{\nu_n + \bar{\nu}_m} \tag{4}$$

holds for the eigenstates $\{|\chi_n\rangle\}$ of $\hat{K}^\dagger$.

With the aid of the conjugate basis $\{|\chi_n\rangle\}$, we can show that the eigenstates $\{|\phi_n\rangle\}$ of $\hat{K}$, although not orthogonal, are nevertheless linearly independent.

This follows from the biorthogonality relation

$$\langle \chi_n | \phi_m \rangle = \delta_{nm} \langle \chi_n | \phi_n \rangle. \tag{5}$$

To see this, we note that by definitions (1) and (2) we have

$$\langle \chi_m | \hat{K} | \phi_n \rangle = \bar{\nu}_m \langle \chi_m | \phi_n \rangle = \kappa_n \langle \chi_m | \phi_n \rangle. \tag{6}$$

Hence $\langle \chi_m | \phi_n \rangle = 0$ if $\kappa_n \neq \bar{\nu}_m$, and $\kappa_n = \bar{\nu}_m$ if $\langle \chi_m | \phi_n \rangle \neq 0$.

Since $\langle \chi_m | \phi_n \rangle = 0$ cannot hold for all $\{|\chi_m\rangle\}$, there has to be at least one ν_m such that $\kappa_n = \bar{\nu}_m$.

On the other hand, by assumption the eigenvalues are not degenerate, so there cannot be more than one ν_m for which $\kappa_n = \bar{\nu}_m$.

The linear independence implies that $\{|\phi_n\rangle\}$ forms a *complete* set of basis for $\mathcal{H}$.

Additionally, they are *minimal* in that exclusion of any one of the elements $|\phi_k\rangle$ from the set $\{|\phi_n\rangle\}$ spoils completeness.

A set of basis elements that is both minimal and complete is called *exact*.

In finite dimensions, the exactness of $\{|\phi_n\rangle\}$ implies the exactness of $\{|\chi_n\rangle\}$, whereas in infinite dimensions this no longer is the case.

Using the independence of the states $\{|\phi_n\rangle\}$ we can establish

$$\sum_n \frac{|\phi_n\rangle\langle\chi_n|}{\langle\chi_n|\phi_n\rangle} = \mathbb{1}. \tag{7}$$

This holds in finite dimensions away from degeneracies.

To show this, note that if $\langle\psi|\hat{F}|\psi\rangle = \langle\psi|\psi\rangle$ for any $|\psi\rangle$, then $\hat{F} = \mathbb{1}$.

Writing $|\psi\rangle = \sum_m c_m|\phi_m\rangle$ for some $\{c_m\}$ we have

$$\langle\psi|\left(\sum_n \frac{|\phi_n\rangle\langle\chi_n|}{\langle\chi_n|\phi_n\rangle}\right)|\psi\rangle = \sum_n\sum_m \bar{c}_m c_n\langle\phi_m|\phi_n\rangle = \langle\psi|\psi\rangle, \tag{8}$$

and this establishes the claim.

The operator $\hat{\Pi}_n$ defined by

$$\hat{\Pi}_n = \frac{|\phi_n\rangle\langle\chi_n|}{\langle\chi_n|\phi_n\rangle} \tag{9}$$

thus plays the role of a projection operator satisfying $\hat{\Pi}_n\hat{\Pi}_m = \delta_{nm}\hat{\Pi}_n$.

Although $\hat{\Pi}_n$ is not Hermitian, its eigenvalues are all zero, except one which is unity, for which the eigenstate is $|\phi_n\rangle$.

Writing $\hat{\Phi}_n = |\phi_n\rangle\langle\phi_n|/\langle\phi_n|\phi_n\rangle$ for the eigenstate projector we have

$$\hat{\Pi}_n\hat{\Phi}_n = \hat{\Phi}_n\hat{\Pi}_n = \hat{\Phi}_n. \tag{10}$$

It follows, in particular, that

$$(\mathbb{1} - \hat{\Pi}_n)|\phi_n\rangle = (\mathbb{1} - \hat{\Pi}^\dagger_n)|\chi_n\rangle = 0. \tag{11}$$

While the complex Hamiltonian $\hat{K}$ does not admit the representation $\sum_n \kappa_n \hat{\Phi}_n$, it can be expressed in the form

$$\hat{K} = \sum_n \kappa_n \hat{\Pi}_n. \tag{12}$$

It follows that if we write, for an arbitrary state $|\psi\rangle = \sum_m c_m |\phi_m\rangle$,

$$\psi_n^{\chi} = \frac{\langle \phi_n | \psi \rangle}{\sqrt{\langle \phi_n | \chi_n \rangle}} \quad \text{and} \quad \psi_n^{\phi} = \frac{\langle \chi_n | \psi \rangle}{\sqrt{\langle \chi_n | \phi_n \rangle}}, \tag{13}$$

then we have

$$\langle \varphi | \psi \rangle = \sum_n \bar{\varphi}_n^{\chi} \psi_n^{\phi}. \tag{14}$$

Quantum probabilities

In quantum theory, the norm of a state is closely related to probabilistic interpretations of measurement outcomes.

We fix our norm convention so that it is consistent with probabilistic considerations of a quantum system.

The norm of the eigenvectors are often assumed to take values larger than unity so as to ensure the following relation holds for all n:

$$\langle \chi_n | \phi_n \rangle = 1. \tag{15}$$

Under this convention, eigenvectors will no longer be normalised.

In particular, if we assume that all eigenstates have the same Hermitian norm so that $\langle \phi_n | \phi_n \rangle = \langle \phi_m | \phi_m \rangle$ for all n, m, then we have $\langle \phi_n | \phi_n \rangle \geq 1$.

The convention $\langle \chi_n | \phi_n \rangle = 1$ leads to considerable simplifications.

In standard quantum mechanics, the ‘transition probability’ between a pair of states $|\xi\rangle$ and $|\eta\rangle$ is given by $\langle\xi|\eta\rangle\langle\eta|\xi\rangle/\langle\xi|\xi\rangle\langle\eta|\eta\rangle$.

Under the convention $\langle\chi_n|\phi_n\rangle = 1$, however, we cannot maintain a consistent probabilistic interpretation from this definition.

For instance, if the state of the system is in an eigenstate $|\phi_n\rangle$ of $\hat{K}$, then on account of stationarity there cannot be a ‘transition’ into another state $|\phi_m\rangle$, $m \neq n$, even though $\langle\phi_m|\phi_n\rangle \neq 0$.

To reconcile these apparent contradictions we need the introduction of the so-called associated state that defines duality relations between elements of the Hilbert space $\mathcal{H}$ and its dual space $\mathcal{H}^*$.

For an arbitrary state $|\psi\rangle$, we define the *associated state* $|\tilde{\psi}\rangle$ according to the following relations:

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \quad \Leftrightarrow \quad \langle\tilde{\psi}| = \sum_n \bar{c}_n\langle\chi_n| \quad \Rightarrow \quad |\tilde{\psi}\rangle = \sum_n c_n|\chi_n\rangle. \tag{16}$$

This determines the duality relation: $|\psi\rangle \in \mathcal{H} \Leftrightarrow |\tilde{\psi}\rangle \in \mathcal{H}^*$.

The quantum-mechanical inner product for a biorthogonal system is thus defined as follows:

If $|\psi\rangle = \sum_n c_n|\phi_n\rangle$ and $|\varphi\rangle = \sum_n d_n|\phi_n\rangle$, then

$$\langle\varphi,\psi\rangle \equiv \langle\tilde{\varphi}|\psi\rangle = \sum_{n,m} \bar{d}_n c_m \langle\chi_n|\phi_m\rangle = \sum_n \bar{d}_n c_n. \tag{17}$$

Since we demand the convention that $\langle\chi_n|\phi_n\rangle = 1$ for all n, we can assume that

$$\langle\tilde{\psi}|\psi\rangle = \sum_n \bar{c}_n c_n = 1. \tag{18}$$

It also follows that $p_n = \bar{c}_n c_n$ defines the transition probability between $|\psi\rangle$ and $|\phi_n\rangle$:

$$p_n = \frac{\langle\chi_n|\psi\rangle\langle\tilde{\psi}|\phi_n\rangle}{\langle\tilde{\psi}|\psi\rangle\langle\chi_n|\phi_n\rangle}. \tag{19}$$

The interpretation of the number p_n is as follows.

If a system is in a state characterised by $|\psi\rangle$, and if a measurement is performed on the 'complex observable' $\hat{K}$, then the probability that the measurement outcome taking the value κ_n is given by p_n.

More generally, the overlap distance s between the two states $|\xi\rangle$ and $|\eta\rangle$ will be defined according to the prescription:

$$\cos^2 \tfrac{1}{2}s = \frac{\langle\tilde{\xi}|\eta\rangle\langle\tilde{\eta}|\xi\rangle}{\langle\tilde{\xi}|\xi\rangle\langle\tilde{\eta}|\eta\rangle}. \tag{20}$$

A short exercise making use of the Cauchy-Schwarz inequality shows that the right side of (20) is real, nonnegative, and lies between zero and one, thus qualifying the required probabilistic conditions.

In particular, $s = 0$ only if $|\xi\rangle = |\eta\rangle$; whereas $s = \pi$ only if $\sum_n \bar{c}_n d_n = 0$ where $|\xi\rangle = \sum_n c_n|\phi_n\rangle$ and $|\eta\rangle = \sum_n d_n|\phi_n\rangle$.

In quantum mechanics the notion of probability is closely related to that of distance.

To see this, suppose that $|\eta\rangle = |\xi\rangle + |\mathrm{d}\xi\rangle$ is a neighbouring state to $|\xi\rangle$.

Then we obtain the Fubini-Study line element:

$$\mathrm{d}s^2 = 4\frac{\langle\tilde{\xi}|\xi\rangle\langle\widetilde{\mathrm{d}\xi}|\mathrm{d}\xi\rangle - \langle\tilde{\xi}|\mathrm{d}\xi\rangle\langle\widetilde{\mathrm{d}\xi}|\xi\rangle}{\langle\tilde{\xi}|\xi\rangle^2}. \tag{21}$$

In two dimensions, an arbitrary normalised state $|\xi\rangle$ can be expressed in the form

$$|\xi\rangle = \cos\tfrac{1}{2}\theta|\phi_1\rangle + \sin\tfrac{1}{2}\theta\mathrm{e}^{\mathrm{i}\varphi}|\phi_2\rangle. \tag{22}$$

In this case we deduce

$$\mathrm{d}s^2 = \tfrac{1}{4}\left(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\varphi^2\right). \tag{23}$$

Observables and states

Given a fixed biorthogonal basis $\{|\phi_n\rangle, |\chi_n\rangle\}$, a generic observable $\hat{F}$ can be expressed in the form

$$\hat{F} = \sum_{n,m} f_{nm} |\phi_n\rangle\langle\chi_m|. \tag{24}$$

If $\hat{G}$ is another observable with 'matrix' elements g_{nm} in the basis $\{|\phi_n\rangle, |\chi_n\rangle\}$, then the matrix element of the product $\hat{F}\hat{G}$ is just $\sum_l f_{nl} g_{lm}$.

The expectation value of a generic observable $\hat{F}$ $|\psi\rangle$ is

$$\langle\hat{F}\rangle = \frac{\langle\tilde{\psi}|\hat{F}|\psi\rangle}{\langle\tilde{\psi}|\psi\rangle}. \tag{25}$$

If the array $\{f_{nm}\}$ in (24) is 'biorthogonally Hermitian' in the sense that $\bar{f}_{nm} = f_{mn}$, then $\langle\hat{F}\rangle$ is real for all states $|\psi\rangle$.

Thus, the notion of Hermiticity extends naturally to the biorthogonal setup, and we are able to speak about physical observables in the usual sense.

If we let $|\psi\rangle = \sum_n c_n|\phi_n\rangle$, then

$$\langle \hat{F}\rangle = \frac{\sum_{n,m}\bar{c}_n c_m f_{nm}}{\sum_n \bar{c}_n c_n}. \tag{26}$$

In particular, if $\{|\phi_n\rangle\}$ are eigenstates of $\hat{F}$, then we can write $f_{nm} = f_n\delta_{nm}$, where $\{f_n\}$ are the eigenvalues of $\hat{F}$, hence

$$\langle \hat{F}\rangle = \sum_n p_n f_n, \tag{27}$$

which is consistent with the probabilistic interpretation of the biorthogonal system.

Now suppose that $\{|e_n\rangle\}$ is an orthonormal basis of $\mathcal{H}$ such that

$$|\phi_n\rangle = \sum_k u_n^k|e_k\rangle, \qquad |\chi_n\rangle = \sum_k v_n^k|e_k\rangle. \tag{28}$$

Then the matrix element of the observable $\hat{F}$ in this orthonormal basis is

$$\hat{F} = \sum_{n,m}\left(\sum_{k,l} f_{kl}u_k^n\bar{v}_l^m\right)|e_n\rangle\langle e_m|. \tag{29}$$

In this way we see more explicitly that while the reality of $\hat{F}$ merely requires Hermiticity of $\{f_{nm}\}$, the Hermiticity of $\hat{F}$ requires a more stringent condition that

$$\sum_{k,l} f_{kl} u_k^n \bar{v}_l^m = \sum_{k,l} \bar{f}_{kl} \bar{u}_k^m v_l^n. \tag{30}$$

In particular, if $\hat{F}$ is Hermitian so that $\hat{F}^\dagger = \hat{F}$, then $\{|e_n\rangle\}$ can be chosen to be $|\phi_n\rangle$ so that $u_k^n = v_k^n = \delta_k^n$ and (30) reduces to the familiar condition $f_{nm} = \bar{f}_{mn}$.

If $\hat{F}$ is symmetric, then we have $v_k^n = \bar{u}_k^n$, i.e. components of $|\chi_n\rangle$ are complex conjugates of the components of $|\phi_n\rangle$.

The expansion coefficients $\{u_k^n\}$ are unique up to unitary transformations.

The linear independence of $\{|\phi_n\rangle\}$ implies that $\{u_n^k\}$ is invertible, and the orthonormality condition $\langle\chi_n|\phi_m\rangle = \delta_{nm}$ implies that the inverse of $\{u_n^k\}$ is given by $\{\bar{v}_n^k\}$.

Phrased differently, if we write $|\phi_n\rangle = \hat{u}|e_n\rangle$ and $|\chi_n\rangle = \hat{v}|e_n\rangle$, then we have $\hat{v}^\dagger\hat{u} = \mathbb{1}$.

If $\hat{F}$ is real (biorthogonally Hermitian), then

$$\hat{F}^\dagger = \hat{v}\hat{v}^\dagger\,\hat{F}\,\hat{u}\hat{u}^\dagger = (\hat{u}\hat{u}^\dagger)^{-1}\hat{F}\,(\hat{u}\hat{u}^\dagger), \tag{31}$$

where $\hat{u}\hat{u}^\dagger$ is an invertible positive Hermitian operator.

As an elementary illustrative example, consider the complex 2×2 Hamiltonian

$$\hat{K} = \hat{\sigma}_x - \mathrm{i}\gamma\hat{\sigma}_z \qquad (\gamma^2 < 1). \tag{32}$$

A calculation shows that the eigenstates of $\hat{K}$ and $\hat{K}^\dagger$, in the region $\gamma^2 < 1$ for which the eigenvalues $\pm\sqrt{1-\gamma^2}$ are real, are given by

$$|\phi_\pm\rangle = n_\pm\begin{pmatrix} 1 \\ \mathrm{i}\gamma \pm \sqrt{1-\gamma^2}\end{pmatrix}, \qquad |\chi_\pm\rangle = n_\mp\begin{pmatrix} 1 \\ -\mathrm{i}\gamma \pm \sqrt{1-\gamma^2}\end{pmatrix}, \tag{33}$$

where

$$n_\pm^2 = (1 \mp \mathrm{i}\gamma/\sqrt{1-\gamma^2})/2. \tag{34}$$

An arbitrary observable for which the expectation value is *real* can be expressed, up to trace, as a linear combination of the deformed Pauli matrices

$$\hat{\sigma}_x^\gamma = \frac{1}{\sqrt{1-\gamma^2}}\begin{pmatrix} -\mathrm{i}\gamma & 1 \\ 1 & \mathrm{i}\gamma \end{pmatrix}, \quad \hat{\sigma}_y^\gamma = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \hat{\sigma}_z^\gamma = \frac{1}{\sqrt{1-\gamma^2}}\begin{pmatrix} 1 & \mathrm{i}\gamma \\ \mathrm{i}\gamma & -1 \end{pmatrix}. \tag{35}$$

The expectation values of these Pauli matrices in a generic state

$$|\xi\rangle = \cos\tfrac{1}{2}\theta|\phi_+\rangle + \sin\tfrac{1}{2}\theta\mathrm{e}^{\mathrm{i}\varphi}|\phi_-\rangle. \tag{36}$$

are then given by

$$\langle\hat{\sigma}_x^\gamma\rangle = \sin\theta\cos\varphi, \quad \langle\hat{\sigma}_y^\gamma\rangle = \sin\theta\sin\varphi, \quad \langle\hat{\sigma}_z^\gamma\rangle = \cos\theta. \tag{37}$$

Note that the right-sides of these expectation values are independent of γ, on account of the γ-dependence of the eigenstates.

Perturbation analysis

Consider now the perturbation analysis involving complex Hamiltonians, in the range where there are no degeneracies so that the Rayleigh-Schrödinger series is applicable.

Let $\hat{K}$ be a complex Hamiltonian with distinct eigenvalues $\{\kappa_n\}$ and biorthonormal eigenstates $(\{|\phi_n\rangle\}, \{|\chi_n\rangle\})$ that are known.

Suppose that we perturb the Hamiltonian slightly according to

$$\hat{K} \longrightarrow \hat{K}_\epsilon = \hat{K} + \epsilon \hat{K}', \tag{38}$$

where $\epsilon \ll 1$ is the perturbation parameter, and $\hat{K}'$ represents perturbation energy, which may or may not be Hermitian.

Under the assumption of no degeneracies, the eigenstates $\{|\psi_n\rangle\}$ and the eigenvalues $\{\mu_n\}$ of $\hat{K}_\epsilon$ can be expanded in a power series

$$|\psi_n\rangle = |\phi_n\rangle + \epsilon|\psi_n^{(1)}\rangle + \epsilon^2|\psi_n^{(2)}\rangle + \cdots , \qquad \mu_n = \kappa_n + \epsilon\mu_n^{(1)} + \epsilon^2\mu_n^{(2)} + \cdots . \tag{39}$$

Since $\langle \chi_n | \phi_n \rangle = 1$, it follows that under this normalisation convention we require

$$\langle \chi_n | \psi_n^{(1)} \rangle = \langle \chi_n | \psi_n^{(2)} \rangle = \cdots = 0. \tag{40}$$

If we substitute the series expansion in the eigenvalue equation

$$\hat{K}_\epsilon | \psi_n \rangle = \mu_n | \psi_n \rangle \tag{41}$$

and equate terms of different orders in ϵ, then we obtain

$$(\kappa_n - \hat{K}) | \phi_n \rangle = 0, \qquad (\kappa_n - \hat{K}) | \psi_n^{(1)} \rangle + \mu_n^{(1)} | \phi_n \rangle = \hat{K}' | \phi_n \rangle, \tag{42}$$

and so on.

Transvecting $\langle \chi_m |$ from the left on the second equation of (42) we obtain

$$(\kappa_n - \kappa_m) \langle \chi_m | \psi_n^{(1)} \rangle + \mu_n^{(1)} \delta_{nm} = \langle \chi_m | \hat{K}' | \phi_n \rangle. \tag{43}$$

Thus, for $n = m$ we obtain the first-order perturbation correction to the eigenvalue:

$$\mu_n^{(1)} = \langle \chi_n | \hat{K}' | \phi_n \rangle. \tag{44}$$

On the other hand, for $n \neq m$ we obtain

$$\langle \chi_m | \psi_n^{(1)} \rangle = \frac{1}{\kappa_n - \kappa_m} \langle \chi_m | \hat{K}' | \phi_n \rangle, \tag{45}$$

and on account of the completeness condition we thus find

$$|\psi_n^{(1)}\rangle = \sum_m |\phi_m\rangle\langle\chi_m|\psi_n^{(1)}\rangle = \sum_{m\neq n} |\phi_m\rangle\langle\chi_m|\psi_n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle\chi_m|\hat{K}'|\phi_n\rangle}{\kappa_n - \kappa_m} |\phi_m\rangle, \tag{46}$$

where we have made use of the orthogonality relations.

In the case of a Hermitian operator, a theorem of Rellich implies that the eigenstates and eigenvalues can be expanded in a Taylor series.

For a general complex operator, the above perturbation expansion breaks down in the vicinities of degeneracies where not only the eigenvalues but also the corresponding eigenstates coalesce.

Dynamics

Consider the evolution operator

$$\hat{U} = \mathrm{e}^{-\mathrm{i}\hat{K}t}, \tag{47}$$

in units $\hbar = 1$.

Evidently, $\hat{U}$ is not unitary: $\hat{U}^\dagger \hat{U} \neq \mathbb{1}$.

However, if the eigenvalues of $\hat{K}$ are real, then $\hat{U}$ in effect is unitary in the sense of biorthogonal quantum mechanics.

It should be apparent that the solution to the dynamical equation

$$\mathrm{i}\partial_t |\psi\rangle = \hat{K}|\psi\rangle, \tag{48}$$

with initial condition $|\psi_0\rangle = \sum_n c_n |\phi_n\rangle$, is given by

$$|\psi_t\rangle = \sum_n c_n \mathrm{e}^{-\mathrm{i}\kappa_n t} |\phi_n\rangle. \tag{49}$$

According to our conjugation rule we have

$$\langle\tilde{\psi}_t| = \sum_n \bar{c}_n \mathrm{e}^{\mathrm{i}\bar{\kappa}_n t}\langle\chi_n| \quad \Rightarrow \quad |\tilde{\psi}_t\rangle = \sum_n c_n \mathrm{e}^{-\mathrm{i}\kappa_n t}|\chi_n\rangle. \tag{50}$$

The time-dependent biorthogonal norm of the state therefore is given by

$$\langle\tilde{\psi}_t|\psi_t\rangle = \sum_n \bar{c}_n c_n \mathrm{e}^{-\mathrm{i}(\kappa_n-\bar{\kappa}_n)t}. \tag{51}$$

Therefore, if the eigenvalues of $\hat{K}$ are real so that $\bar{\kappa}_n = \kappa_n$, then for all time $t > 0$ we have $\langle\tilde{\psi}_t|\psi_t\rangle = \langle\tilde{\psi}_0|\psi_0\rangle$.

More generally, if $\bar{\kappa}_n = \kappa_n$, and if $|\varphi_t\rangle$ is also a solution to the Schrödinger equation with a different initial condition, then for all $t > 0$

$$\langle\tilde{\varphi}_t|\psi_t\rangle = \langle\tilde{\varphi}_0|\psi_0\rangle. \tag{52}$$

It follows that:

Proposition 1. *If the eigenvalues of $\hat{K}$ are real, then the time evolution operator $\mathrm{e}^{-\mathrm{i}\hat{K}t}$ is unitary with respect to the biorthogonal basis of $\hat{K}$, preserving the biorthogonal norms of the states and the transition probabilities between states.*

When one or more of the eigenvalues are imaginary or complex, we have different characteristics for the dynamical behaviour.

Let us write

$$\kappa_n = E_n - \mathrm{i}\gamma_n \tag{53}$$

for the eigenvalues, where $\{E_n\}$ and $\{\gamma_n\}$ are real.

Then we have

$$\langle\tilde{\psi}_t|\psi_t\rangle = \sum_n \bar{c}_n c_n \mathrm{e}^{-2\gamma_n t} = \bar{c}_{n_*} c_{n_*} \mathrm{e}^{-2\gamma_{n_*} t}\left(1 + \sum_{n\neq n_*} \frac{\bar{c}_n c_n}{\bar{c}_{n_*} c_{n_*}}\, \mathrm{e}^{-2(\gamma_n - \gamma_{n_*})t}\right), \tag{54}$$

where n_* is the value of n such that γ_n has the smallest value.

In most physical setups, $\gamma_n \geq 0$, and an arbitrary initial state will decay into the state with the smallest γ_n value.

This situation describes the behaviour of a particle trapped in a finite potential well; the norm $\langle\tilde{\psi}_t|\psi_t\rangle$ then describes the probability that the particle has not tunnelled out of the well.

Relation to PT symmetry

If we write $\hat{g} = (\hat{u}\hat{u}^\dagger)^{-1}$, then on account of

$$|\phi_n\rangle = \sum_k u_n^k |e_k\rangle, \qquad |\chi_n\rangle = \sum_k v_n^k |e_k\rangle \tag{55}$$

we have

$$\langle e_n|e_n\rangle = \langle \phi_n|\hat{g}|\phi_n\rangle \tag{56}$$

for all n.

Here $\hat{g}$ by construction is an invertible positive Hermitian operator, which is unique and can be determined from the eigenstates:

$$\hat{g}^{-1} = \sum_n |\phi_n\rangle\langle\phi_n|. \tag{57}$$

In addition, observe, for all n, that

$$\langle \phi_n|\hat{g}^2|\phi_n\rangle = \langle e_n|(\hat{u}^{-1})^\dagger \hat{u}^{-1}(\hat{u}^{-1})^\dagger \hat{u}^{-1}|e_n\rangle = \langle e_n|\hat{u}^{-1}(\hat{u}^{-1})^\dagger|e_n\rangle = \langle \chi_n|\chi_n\rangle, \tag{58}$$

but $\langle \chi_n|\chi_n\rangle = \langle \phi_n|\phi_n\rangle$, so $\hat{g}$ is an involution:

$$\hat{g}^2 = \mathbb{1}. \tag{59}$$

Perceived from the viewpoint of Hermitian inner-product space, therefore, the operator $\hat{g}$ plays the role of a 'metric' for the Hilbert space.

For example, the expectation value of a physical observable $\hat{F}$ can be written in the form

$$\frac{\langle\tilde{\psi}|\hat{F}|\psi\rangle}{\langle\tilde{\psi}|\psi\rangle} = \frac{\langle\psi|\hat{g}\hat{F}|\psi\rangle}{\langle\psi|\hat{g}|\psi\rangle} \qquad (60)$$

that involves the metric operator under the Hermitian pairing.

We see therefore that biorthogonal quantum mechanics can alternatively be viewed as 'conventional' Hermitian quantum mechanics, but where Hilbert space is endowed with a nontrivial metric operator $\hat{g}$.

This metric is the so-called "metric operator" in PT-symmetric quantum theory.

Complex degeneracies:

In the case of a Hermitian Hamiltonian, the first-order perturbation breaks down near degeneracies, and one has to consider higher orders.

In the case of a complex Hamiltonian, the situation is more severe on account of the fact that the Rayleigh-Schrödinger perturbation theory breaks down altogether in the vicinities of exceptional points.

Nevertheless, for a given Hamiltonian one can expand the eigenstates and eigenvalues in the form of Newton-Puiseux series.

Let us illustrate how such an analysis can be applied to deduce the nature of geometric singularities close to exceptional points.

At an exceptional point two or more eigenvalues and the corresponding eigenstates coalesce, that is, the Hamiltonian is not diagonalisable.

Here we consider the most common case, where two eigenvalues and the corresponding eigenstates coalesce.

At such an exceptional point there is a two-fold degenerate eigenvalue κ_{EP} and a single eigenvector $|\phi_{EP}\rangle$, which is orthogonal to the corresponding left eigenvector: $\langle\chi_{EP}|\phi_{EP}\rangle = 0$.

However, one can define an associated vector, the so-called Jordan vector, denoted $|\phi^J_{EP}\rangle$, fulfilling the relation

$$\hat{K}|\phi^J_{EP}\rangle = \kappa_{EP}|\phi^J_{EP}\rangle + |\phi_{EP}\rangle. \tag{61}$$

Similarly the left Jordan vector can be defined according to the relation

$$\hat{K}^\dagger|\chi^J_{EP}\rangle = \bar{\kappa}_{EP}|\chi^J_{EP}\rangle + |\chi_{EP}\rangle. \tag{62}$$

The Jordan vector $|\phi^J_{EP}\rangle$ and the eigenvector $|\phi_{EP}\rangle$ span the two-dimensional eigenspace corresponding to the degenerate eigenvalue κ_{EP}.

Note that the Jordan vector is not uniquely defined by equation (61).

However, the ambiguity can be removed by choosing appropriate normalisation conditions.

In fact, it will be convenient to normalise the states such that

$$\langle \chi_{EP} | \phi_{EP}^{J} \rangle = \langle \chi_{EP}^{J} | \phi_{EP} \rangle = 1, \tag{63}$$

and that

$$\langle \chi_{EP}^{J} | \phi_{EP}^{J} \rangle = 0. \tag{64}$$

The conventional Rayleigh-Schrödinger perturbation theory breaks down around an exceptional point, and in general the eigenvalues and eigenvectors are not analytic functions of the perturbation parameter.

That is, they cannot be expanded in a Taylor series.

In the general case they can nevertheless be expanded into a power series with broken rational exponents, which is known as a Puiseux series.

The most common behaviour around an exceptional point at which two eigenvectors coalesce is that the eigenvalues and eigenvectors can be expanded in a power series with half-integral exponents.

Let $\epsilon \ll 1$ denote a small perturbation parameter that measures the deviation away from the exceptional point.

Expanding the Hamiltonian, the eigenvalues and eigenvectors in lowest order in ϵ in the eigenvalue equation yields

$$(\hat{K}_{EP}+\epsilon\hat{K}'+\cdots)(|\phi_{EP}\rangle+|\phi'\rangle\epsilon^{\frac{1}{2}}+\cdots)=(\kappa_{EP}+\kappa'\epsilon^{\frac{1}{2}}+\cdots)(|\phi_{EP}\rangle+|\phi'\rangle\epsilon^{\frac{1}{2}}+\cdots) \tag{65}$$

Equating terms corresponding to different powers of ϵ we find that the two eigenstates $|\phi_\pm\rangle$ can be expanded in the form:

$$|\phi_\pm\rangle = n\Big(|\phi_{EP}\rangle+\kappa'_\pm\,\epsilon^{\frac{1}{2}}\,|\phi^J_{EP}\rangle+O(\epsilon)\Big), \tag{66}$$

where

$$\kappa'_\pm = \pm\sqrt{\langle\chi_{EP}|\hat{K}'|\phi_{EP}\rangle}. \tag{67}$$

A perturbative expression similar to (66) holds for the left eigenvector.

It is convenient to normalise these vectors according to the usual biorthogonal convention away from the exceptional point: $\langle\chi_\pm|\phi_\pm\rangle=1$.

From this we find that

$$|\phi_\pm\rangle \approx \frac{1}{\sqrt{2\kappa'}\epsilon^{1/4}}\left(|\phi_{EP}\rangle + \kappa'\,\epsilon^{\frac{1}{2}}\,|\phi^J_{EP}\rangle\right) \tag{68}$$

and that

$$\langle\chi_\pm| \approx \frac{1}{\sqrt{2\kappa'}\epsilon^{1/4}}\left(\langle\chi_{EP}| + \kappa'\,\epsilon^{\frac{1}{2}}\,\langle\chi^J_{EP}|\right). \tag{69}$$

A calculation then shows that

$$|\mathrm{d}\phi_+\rangle = \frac{1}{4\sqrt{\kappa'}}\left(-\epsilon^{-\frac{5}{4}}|\phi_{EP}\rangle + \kappa'\,\epsilon^{-\frac{3}{4}}\,|\phi^J_{EP}\rangle\right)\mathrm{d}\epsilon = \frac{1}{4\epsilon}\,|\phi_-\rangle\mathrm{d}\epsilon, \tag{70}$$

and hence that

$$\langle\widetilde{\mathrm{d}\phi_+}| = \frac{1}{4\epsilon}\langle\chi_-|\mathrm{d}\epsilon. \tag{71}$$

From these we thus find the expression of the metric close to an exceptional point of second order where two eigenstates coalesce:

$$G = \frac{1}{4\epsilon^2}. \tag{72}$$

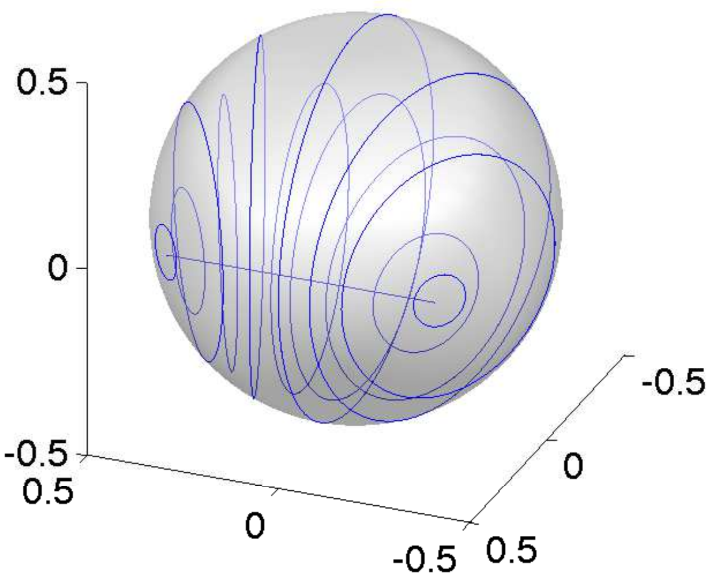
It should be remarked that this result is generic, i.e. it is independent of the model.

Dynamics revisited

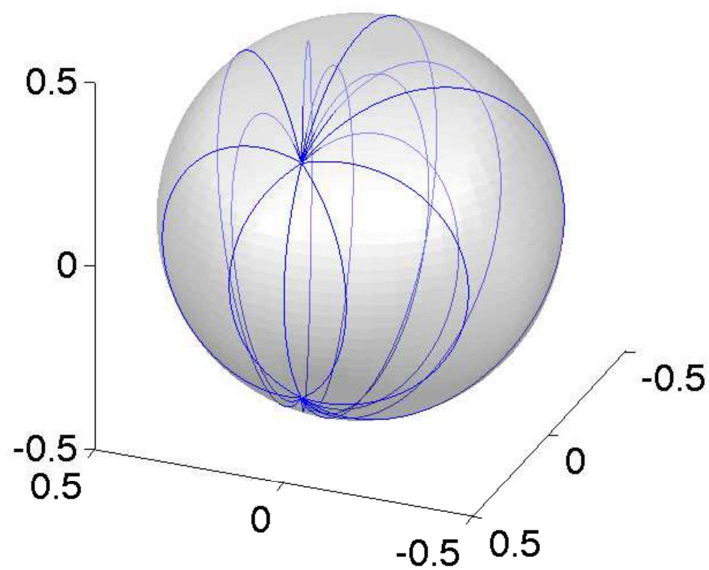
An alternative way of viewing the dynamics is to write

$$\frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = -\mathrm{i}(H - \langle H\rangle)|\psi\rangle - (\Gamma - \langle\Gamma\rangle)|\psi\rangle. \tag{73}$$

As an example consider the Hamiltonian $\hat{K} = \hat{\sigma}_x - \mathrm{i}\hat{\sigma}_z$. Then for the dynamics we have the following.



(a) unbroken phase



(b) broken phase

We can ask if there is an analogue of Wigner's theorem when the generator of the dynamics is not Hermitian.

In this case, an analysis shows that

(a) The resulting motion generates a holomorphic vector field;

(b) Every holomorphic vector field on the state space arises from such a Hamiltonian;

(c) The symmetry group of the motion is that associated with holomorphically projective transformations that map complex geodesics to complex geodesics; and

(d) Every map that preserves complex geodesics on the state space must arise from a Hamiltonian $\hat{K}$ that is not necessarily Hermitian.

Towards infinite dimensions

Already in quantum mechanics based on conventional Hermitian operators there are subtleties in going from finite to infinite-dimensional Hilbert spaces.

It should be clear that the matter does not improve when considering quantum mechanics beyond Hermitian operators.

Indeed, the following simple example illustrates how a completeness statement of biorthogonal quantum mechanics that holds true in finite dimensions can easily fail in infinite dimensions.

Consider an infinite-dimensional Hilbert space $\mathcal{H}$ and an orthonormal set of basis $\{|e_n\rangle\}$ in $\mathcal{H}$.

Construct a new set of basis elements $\{|\phi_n\rangle\}$ according to

$$|\phi_n\rangle = |e_1\rangle + |e_n\rangle \tag{74}$$

for $n = 2, 3, \ldots, \infty$.

Elements of $\{|\phi_n\rangle\}$ are not orthogonal, but the set is complete:

$$\lim_{N\to\infty} \frac{1}{N-1} \sum_{n=2}^{N} |\phi_n\rangle = |e_1\rangle + \lim_{N\to\infty} \frac{1}{N-1} \sum_{n=2}^{N} |e_n\rangle = |e_1\rangle. \tag{75}$$

The biorthogonal pair of $|\phi_n\rangle$ is unique and is given by

$$|\chi_n\rangle = |e_n\rangle \tag{76}$$

for $n = 2, 3, \ldots, \infty$.

So we have $\langle \chi_n | \phi_m \rangle = \delta_{nm}$.

While the set $\{|\phi_n\rangle\}$ is complete, its biorthogonal counterpart $\{|\chi_n\rangle\}$ is not—a phenomenon that has no analogue in finite dimensions.

Thus, if $\hat{K} = \sum_n \kappa_n |\phi_n\rangle\langle\chi_n|$ is a Hamiltonian operator acting on the states of $\mathcal{H}$, then we can form a linear combination of the eigenstates of $\hat{K}$ that has a null conjugate state:

$$\langle \tilde{e}_1 | e_1 \rangle = 0. \tag{77}$$

If we interpret the norm as representing the probability of finding a particle in the system, then we have a 'no-particle' state $|e_1\rangle$ that nevertheless has nonzero energy expectation value.

Even if a biorthonormal set $(\{|\phi_n\rangle\}, \{|\chi_n\rangle\})$ is complete, there can be various subtleties arising from the lack of a bounded map that takes an element $|\phi_n\rangle$ into $|e_n\rangle$.

Specifically, suppose that $(\{|\phi_n\rangle\}, \{|\chi_n\rangle\})$ is a complete biorthonormal set of bases in $\mathcal{H} = \mathcal{L}^2$ of square-integrable functions.

Then the set $\{|\phi_n\rangle\}$ is called a 'Fischer-Riesz' basis if

(a) for any $|\psi\rangle \in \mathcal{H}$ we have $\sum_n |\langle\chi_n|\psi\rangle|^2 < \infty$; and

(b) if for any sequence $\{c_n\}$ such that $\sum_n |c_n|^2 < \infty$ there exists a $|\psi\rangle \in \mathcal{H}$ for which $\langle\chi_n|\psi\rangle = c_n$.

A theorem of Bari then shows that:

(i) $\{|\chi_n\rangle\}$ is a Fischer-Riesz basis if and only if there exists a bounded invertible linear operator $\hat{u}^{-1}$ and a complete orthonormal basis elements $\{|e_n\rangle\}$ in $\mathcal{H}$ such that $\hat{u}^{-1}|\phi_n\rangle = |e_n\rangle$; and that

(ii) $\{|\phi_n\rangle\}$ is a Fischer-Riesz basis if and only if there exists a positive bounded invertible linear operator $\hat{g}^{-1}$ in $\mathcal{H}$ such that $|\phi_n\rangle = \hat{g}^{-1}|\chi_n\rangle$.

In infinite dimensions, a generic complex Hamiltonian $\hat{K}$ possessing real eigenvalues often do not admit an invertible bounded metric operator $\hat{g}$.

This implies that a system described by such a Hamiltonian is intrinsically different from that described by a Hermitian Hamiltonian, even if the eigenvalues coincide.

But sometimes one can find interesting nontrivial examples where these conditions are satisfied.

Consider the Hamiltonian

$$\hat{H} = \frac{\mathbb{1}}{\mathbb{1} - \mathrm{e}^{-\mathrm{i}\hat{p}}} \left(\hat{x}\hat{p} + \hat{p}\hat{x}\right) \left(\mathbb{1} - \mathrm{e}^{-\mathrm{i}\hat{p}}\right) \tag{78}$$

defined on $\mathcal{L}^2(\mathbb{R}_+)$.

The eigenfunctions of $\hat{H}$ are given by

$$\psi_n(x) = -\zeta(z_n, x+1) \tag{79}$$

and the eigenvalues are given by

$$E_n = \mathrm{i}(2z_n - 1), \tag{80}$$

where $\zeta(z, x)$ is the Hurwitz zeta function, and z_n are the nontrivial zeros of the Riemann zeta function on the critical line.

In this example, we can show that the transformation operator $(\mathbb{1} - \mathrm{e}^{-\mathrm{i}\hat{p}})^{-1}$ is bounded and invertible.

It then follows that $\hat{H}$ is self-adjoint, i.e. its eigenvalues are real.

References

Bender, C.M., Brody, D.C. & Jones, H.F. (2002) “Complex extension of quantum mechanics” *Physical Review Letters*, **89**, 27040.

Brody, D.C. & Graefe, E.M. (2012) “Mixed-state evolution in the presence of gain and loss” *Physical Review Letters* **109**, 230405.

Brody, D.C. (2013) “Geometry of the complex extension of Wigner’s theorem” *Journal of Physics* A**46**, 395301.

Brody, D.C. (2014) “Biorthogonal quantum mechanics” *Journal of Physics* A**47**, 035305.

Brody, D.C. (2016) “Consistency of PT-symmetric quantum mechanics” *Journal of Physics* A**49**, 10LT03.

Bender, C.M., Brody, D.C. & Müller, M. P. (2017) “Hamiltonian for the zeros of the Riemann zeta function” *Physical Review Letters* **118**, 130201.

