Description of resonances within the rigged Hilbert space

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Abstract. The spectrum of a quantum system has in general bound, scattering and resonant parts. The Hilbert space includes only the bound and scattering spectra, and discards the resonances. One must therefore enlarge the Hilbert space to a rigged Hilbert space, within which the physical bound, scattering and resonance spectra are included on the same footing. In these lectures, I will explain how this is done.

Keywords: Resonances; Hilbert space; rigged Hilbert space; Gamow states
PACS: 03.65.-w, 02.30.Hq

INTRODUCTION: LECTURE 1

In Quantum Mechanics, observable quantities are represented by linear operators. The eigenvalues of an operator represent the possible values of the measurement of the corresponding observable. These eigenvalues, which mathematically correspond to the spectrum of the operator, can be discrete (as the energies of a particle in a box), continuous (as the energies of a free, unconstrained particle), resonant (as in α decay), or a combination thereof.

The Hilbert space includes only the bound and scattering spectra, because the Hilbert space spectrum of an observable is real, thereby discarding the resonance spectrum as unphysical. However, radioactive nuclei and unstable elementary particles are physical objects that ought to have a place in the quantum mechanical formalism. This is why we need to extend the Hilbert space to a rigged Hilbert space, within which the resonance spectrum has a place.

The purpose of this series of lectures is to explain how one should use the rigged Hilbert space in quantum mechanics and, in particular, how to incorporate the resonance spectrum into the quantum mechanical formalism by using the rigged Hilbert space.

When the spectrum of an observable A is discrete and A is bounded, then A is defined on the whole of the Hilbert space $\mathscr{H}$ and the eigenvectors of A belong to $\mathscr{H}$. In this case, A can be essentially seen as a matrix. This means that, as far as discrete spectrum is concerned, there is no need to extend $\mathscr{H}$. However, quantum mechanical observables are in general unbounded and their spectrum has in general a continuous part. In order to deal with continuous spectrum, we use Dirac's bra-ket formalism. This formalism does not fit within the Hilbert space alone, but within the rigged Hilbert space.

Loosely speaking, a rigged Hilbert space (also called a Gelfand triplet) is a triad of spaces

$$\Phi \subset \mathscr{H} \subset \Phi^{\times} \tag{1}$$

such that $\mathscr{H}$ is a Hilbert space, Φ is a dense subspace of $\mathscr{H}$, and $\Phi^\times$ is the space of antilinear functionals over Φ. Mathematically, Φ is the space of test functions, and $\Phi^\times$ is the space of distributions. The space $\Phi^\times$ is called the antidual space of Φ. Associated with the rigged Hilbert space (1), there is always another rigged Hilbert space,

$$\Phi \subset \mathscr{H} \subset \Phi' , \tag{2}$$

where Φ' is called the dual space of Φ and contains the linear functionals over Φ.

The basic reason why we need the spaces Φ' and $\Phi^\times$ is that the bras and kets associated with the elements in the continuous spectrum of an observable belong, respectively, to Φ' and $\Phi^\times$ rather than to $\mathscr{H}$. The basic reason reason why we need the space Φ is that unbounded operators are not defined on the whole of $\mathscr{H}$ but only on dense subdomains of $\mathscr{H}$ that are not invariant under the action of the observables. Such non-invariance makes expectation values, uncertainties and commutation relations not well defined on the whole of $\mathscr{H}$. The space Φ is the largest subspace of the Hilbert space on which such expectation values, uncertainties and commutation relations are well defined.

Besides accommodating resonances and Dirac's bra-ket formalism, the rigged Hilbert space seems to capture the physical principles of quantum mechanics better than the Hilbert space. For example, assuming that the Hilbert space provides the whole mathematical framework for quantum mechanics leads to the conclusion that Heisenberg's uncertainty relations are not physical, since they cannot be defined on the whole of the Hilbert space [1]. Using the rigged Hilbert space, one overcomes this difficulty after realizing that the commutation relations are well defined on Φ.

The completeness relation is a good place to appreciate the added value of the rigged Hilbert space. Consider, for example, the Hamiltonian H of a system. In the Hilbert space, one writes the completeness relation as

$$1 = \int_{\mathrm{Sp}(H)} d\mathsf{E}_E \, , \tag{3}$$

where E_E are the spectral projections of H and $\mathrm{Sp}(H)$ is its spectrum. However, within the rigged Hilbert space one can write[1]

$$1 = \sum_n |E_n\rangle\langle E_n| + \int_0^\infty dE\, |E\rangle\langle E| \, , \tag{4}$$

where $|E_n\rangle$ and $|E\rangle$ are the bound and scattering states of H, respectively. In addition to (4), the rigged Hilbert space gives you an additional completeness relation in which the resonance states participate:

$$1 = \sum_n |E_n\rangle\langle E_n| + \sum_n |z_n\rangle\langle z_n| + \int_{-\infty}^0 dE\, |E\rangle\langle E| \, , \tag{5}$$

where $|z_n\rangle$ are the Gamow (resonance) states of H and the last integral, called the background, is performed in the complex plane right below the negative real axis of the

[1] In the Hilbert space, one can actually write something close to, although not the same as (4), by means of direct integral decompositions.

second sheet.[2] Thus, the completeness relation (5) substitutes the scattering states contribution by the resonance contribution plus a background, thereby putting the resonance spectrum on the same footing as the bound and scattering spectra.

It is important to note that the integrals in (4) and (5) are different, and that the resonance contribution does not appear in (4), because resonances are not asymptotic states. Also important is to note that the resonance states, and therefore expansion (5), need a different rigged Hilbert space from that needed by the scattering states and expansion (4).

There are dangers in using the rigged Hilbert space indiscriminately, though. For instance, A. Bohm and collaborators have been using a rigged Hilbert space (of Hardy class) to construct a quantum theory of resonances, see review [2] and references therein. However, such theory is inconsistent with quantum mechanics and must be discarded [3].

The structure of these lectures is as follows. After an introductory Lecture 1, I will explain in Lecture 2 how to construct the rigged Hilbert space of the one-dimensional rectangular barrier potential. This will show that the rigged Hilbert space is already needed to provide the mathematical support of the most basic quantum systems. In Lecture 3, I will construct the rigged Hilbert space of the Lippmann-Schwinger equation, which equation governs quantum scattering. In Lecture 4, I will construct the rigged Hilbert space of the analytic continuation of the Lippmann-Schwinger equation. The rigged Hilbert space of Lecture 4 will be needed in the final Lecture 5 to provide the mathematical support for the resonance states. The PDF file of each talk will be posted at `http://www.ucsd.edu/~rafa`.

Since space prevents a full account, at each lecture I will refer the reader to the appropriate papers where further details can be found. The essentials of functional analysis needed to understand those papers can be found in [4, Chapter 2].

CONSTRUCTION OF A SIMPLE RIGGED HILBERT SPACE: LECTURE 2

If resonances are not included, the way to construct the rigged Hilbert space of a quantum system is as follows:

1. We identify the observables of the system. Their expressions are usually given by linear, differential operators.
2. We identify the Hilbert space, whose scalar product is used to calculate probability amplitudes.
3. We identify the domains, spectra and eigenfunctions of the observables. If the observables have a discrete spectrum, we need not go beyond the Hilbert space. However, if at least one of the observables has continuous spectrum, we need to enlarge the Hilbert space to the rigged Hilbert space. (If position and momentum

[2] As we will see in Lecture 5, the expansion (5) must be either regulated or understood in a time-dependent way.

are among the observables, we will always need the rigged Hilbert space.)

4. We construct the space Φ in which physical quantities such as expectation values, uncertainties and commutation relations are well defined. When resonances are not included, the space Φ is usually given by the maximal invariant subspace of the algebra of observables.
5. We construct the dual Φ' and antidual $\Phi^{\times}$ spaces. We construct the bras and kets of the observables and check that they respectively belong to Φ' and $\Phi^{\times}$.
6. The completeness relations and all the features of Dirac's bra-ket formalism now follow.

Let's see how the above steps are carried out in the case of a spinless particle moving in one dimension and impinging on a rectangular barrier. The observables relevant to this system are the position Q, the momentum P, and the Hamiltonian H:

$$Qf(x) = xf(x)\,, \tag{6}$$

$$Pf(x) = -i\hbar\frac{d}{dx}f(x)\,, \tag{7}$$

$$Hf(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)f(x)\,, \tag{8}$$

where

$$V(x) = \begin{cases} 0 & -\infty < x < a \\ V_0 & a < x < b \\ 0 & b < x < \infty \end{cases} \tag{9}$$

is the 1D rectangular barrier potential. These observables satisfy the following commutation relations:

$$[Q,P] = i\hbar I\,, \tag{10}$$

$$[H,Q] = -\frac{i\hbar}{m}P\,, \tag{11}$$

$$[H,P] = i\hbar\frac{\partial V}{\partial x}\,. \tag{12}$$

Since our particle can move in the full real line, the Hilbert space on which the differential operators (6)-(8) should act is

$$L^2 = \{f(x)\,|\, \int_{-\infty}^{\infty} dx\,|f(x)|^2 < \infty\}\,. \tag{13}$$

The corresponding scalar product is

$$(f,g) = \int_{-\infty}^{\infty} dx\,\overline{f(x)}g(x)\,, \qquad f,g \in L^2\,. \tag{14}$$

The differential operators (6)-(8) induce three linear operators on the Hilbert space L^2. These operators cannot be defined on the whole of L^2, but only on the following subdomains of L^2:

$$\mathscr{D}(Q) = \left\{f \in L^2 \,|\, xf \in L^2\right\}\,, \tag{15}$$

$$\mathscr{D}(P) = \left\{ f \in L^2 \mid f \in AC,\ Pf \in L^2 \right\} , \tag{16}$$

$$\mathscr{D}(H) = \left\{ f \in L^2 \mid f \in AC^2,\ Hf \in L^2 \right\} , \tag{17}$$

where, essentially, AC is the space of functions whose derivative exists, and AC^2 is the space of functions whose second derivative exists. On these domains, the operators Q, P and H are self-adjoint, and their spectra are

$$\mathrm{Sp}(Q) = \mathrm{Sp}(P) = (-\infty, \infty) , \quad \mathrm{Sp}(H) = [0, \infty) , \tag{18}$$

which spectra coincide with those we would expect on physical grounds.

To obtain the eigenfunctions corresponding to each eigenvalue, we have to solve the eigenvalue equation for each observable:

$$x\langle x|x'\rangle = x'\langle x|x'\rangle , \tag{19}$$

$$-i\hbar \frac{d}{dx}\langle x|p\rangle = p\langle x|p\rangle , \tag{20}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right) \langle x|E\rangle = E\langle x|E\rangle . \tag{21}$$

The eigenfunctions of Q are delta functions,

$$\langle x|x'\rangle = \delta(x - x') , \tag{22}$$

those of P are plane waves,

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} , \tag{23}$$

and those of H are given by

$$\langle x|E^+\rangle_{\mathrm{r}} = \left(\frac{m}{2\pi k\hbar^2} \right)^{1/2} \times \begin{cases} T(k)e^{-ikx} & -\infty < x < a \\ A_{\mathrm{r}}(k)^{i\kappa x} + B_{\mathrm{r}}(k)e^{-i\kappa x} & a < x < b \\ R_{\mathrm{r}}(k)e^{ikx} + e^{-ikx} & b < x < \infty , \end{cases} \tag{24}$$

$$\langle x|E^+\rangle_{\mathrm{l}} = \left(\frac{m}{2\pi k\hbar^2} \right)^{1/2} \times \begin{cases} e^{ikx} + R_{\mathrm{l}}(k)e^{-ikx} & -\infty < x < a \\ A_{\mathrm{l}}(k)e^{i\kappa x} + B_{\mathrm{l}}(k)e^{-i\kappa x} & a < x < b \\ T(k)e^{ikx} & b < x < \infty , \end{cases} \tag{25}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}E} , \quad \kappa = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} , \tag{26}$$

and where the coefficients that appear in Eqs. (24)-(25) can be easily found by the standard matching conditions at the discontinuities of the potential. Physically, $\langle x|E^+\rangle_{\mathrm{r}}$ ($\langle x|E^+\rangle_{\mathrm{l}}$) represents a particle of energy E impinging on the barrier from the right (left).

The eigenfunctions (22)-(25) are not square integrable, that is, they do not belong to L^2. Mathematically speaking, this is the reason why they are to be dealt with as distributions (note that all of them except for the delta function are also proper functions).

We now start the construction of the rigged Hilbert space by constructing Φ. The space Φ is given by

$$\Phi = \bigcap_{\substack{n,m=0 \\ A,B=Q,P,H}}^{\infty} \mathscr{D}(A^n B^m) \, . \tag{27}$$

In view of expressions (6)-(8), Φ is simply

$$\begin{aligned} \Phi = \{ \varphi \in L^2 \mid \varphi \in C^\infty(\mathbb{R}),\ \varphi^{(n)}(a) = \varphi^{(n)}(b) = 0\, ,\ n = 0, 1, \ldots \, , \\ P^n Q^m H^l \varphi(x) \in L^2\, ,\ n, m, l = 0, 1, \ldots \} \, , \end{aligned} \tag{28}$$

where $C^\infty(\mathbb{R})$ is the collection of infinitely differentiable functions, and $\varphi^{(n)}$ denotes the nth derivative of φ. From the last condition in Eq. (28), we deduce that the elements of Φ satisfy the following estimates:

$$\|\varphi\|_{n,m,l} \equiv \sqrt{\int_{-\infty}^{\infty} dx \left| P^n Q^m H^l \varphi(x) \right|^2} < \infty , \quad n, m, l = 0, 1, \ldots \, . \tag{29}$$

These estimates mean that the action of any combination of any power of the observables remains square integrable. For this to happen, the functions $\varphi(x)$ must be infinitely differentiable and must fall off at infinity faster than any polynomial. Hence, Φ is a Schwartz-like space.

Because Φ is invariant under the action of the observables,

$$A\,\Phi \subset \Phi , \qquad A = P, Q, H, \tag{30}$$

the expectation values

$$(\varphi, A^n \varphi)\, , \quad \varphi \in \Phi,\ A = P, Q, H,\ n = 0, 1, \ldots \tag{31}$$

are finite, and the commutation relations (10)-(12) are well defined. In particular, Heisenberg's uncertainty principle makes sense on Φ.

The spaces Φ' and $\Phi^\times$ are simply the collection of linear and antilinear functionals over Φ, respectively. By combining the spaces Φ, $\mathscr{H}$, $\Phi^\times$ and Φ', we obtain the rigged Hilbert spaces of our system,

$$\Phi \subset \mathscr{H} \subset \Phi^\times \, , \tag{32}$$

$$\Phi \subset \mathscr{H} \subset \Phi' \, . \tag{33}$$

The space $\Phi^\times$ accommodates the eigenkets $|p\rangle$, $|x\rangle$ and $|E^+\rangle_{\mathrm{l,r}}$ of P, Q and H, whereas Φ' accommodates the eigenbras $\langle p|$, $\langle x|$ and ${}_{\mathrm{l,r}}\langle ^+E|$.

Mathematically, the bras and kets are distributions defined as follows. Given a function $f(x)$ and a space of test functions Φ, the antilinear functional F that corresponds to the function $f(x)$ is an integral operator whose kernel is precisely $f(x)$:

$$F(\varphi) \equiv \int dx\, \overline{\varphi(x)} f(x) \, , \tag{34}$$

and the linear functional $\tilde{F}$ generated by the function $f(x)$ is an integral operator whose kernel is the complex conjugate of $f(x)$:

$$\tilde{F}(\varphi) \equiv \int dx\, \varphi(x)\overline{f(x)}\,. \tag{35}$$

In Dirac's notation, these two equations become

$$\langle\varphi|F\rangle = \int dx\, \langle\varphi|x\rangle\langle x|f\rangle\,, \tag{36}$$

$$\langle F|\varphi\rangle = \int dx\, \langle f|x\rangle\langle x|\varphi\rangle\,. \tag{37}$$

Note that these definitions are very similar, except that the complex conjugation affects either $f(x)$ or $\varphi(x)$, which makes the corresponding functional either linear or antilinear.

Definitions (34) and (35) provide the link between the quantum mechanical formalism and the theory of distributions. In practical applications, what one obtains from the quantum mechanical formalism is the distribution $f(x)$ (in this lecture, the plane waves $\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$, the delta function $\delta(x-x')$ and the eigenfunctions $\langle x|E^+\rangle_{\mathrm{l,r}}$). Once $f(x)$ is given, one can use definitions (34) and (35) to generate the functionals $|F\rangle$ and $\langle F|$. Then, the theory of distributions can be used to obtain the properties of the functionals $|F\rangle$ and $\langle F|$, which in turn yield the properties of the distribution $f(x)$.

By using prescription (34), we can define for each eigenvalue p the eigenket $|p\rangle$ associated with the eigenfunction (23):

$$\langle\varphi|p\rangle \equiv \int_{-\infty}^{\infty} dx\, \overline{\varphi(x)}\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\,, \tag{38}$$

which, using Dirac's notation for the integrand, becomes

$$\langle\varphi|p\rangle \equiv \int_{-\infty}^{\infty} dx\, \langle\varphi|x\rangle\langle x|p\rangle\,. \tag{39}$$

Similarly, for each x, we can define the ket $|x\rangle$ as

$$\langle\varphi|x\rangle \equiv \int_{-\infty}^{\infty} dx'\, \overline{\varphi(x')}\delta(x-x')\,, \tag{40}$$

which, using Dirac's notation for the integrand, becomes

$$\langle\varphi|x\rangle \equiv \int_{-\infty}^{\infty} dx'\, \langle\varphi|x'\rangle\langle x'|x\rangle\,. \tag{41}$$

The definition of the kets $|E^+\rangle_{\mathrm{l,r}}$ that correspond to the Hamiltonian's eigenfunctions (24)-(25) follows the same prescription:

$$\langle\varphi|E^+\rangle_{\mathrm{l,r}} \equiv \int_{-\infty}^{\infty} dx\, \overline{\varphi(x)}\langle x|E^+\rangle_{\mathrm{l,r}}\,, \tag{42}$$

that is,

$$\langle\varphi|E^+\rangle_{\text{l,r}} \equiv \int_{-\infty}^{\infty} dx\, \langle\varphi|x\rangle\langle x|E^+\rangle_{\text{l,r}}\,. \tag{43}$$

One can now show that the definition of the kets $|p\rangle$, $|x\rangle$ and $|E^+\rangle_{\text{l,r}}$ makes sense, and that these kets indeed belong to the space of distributions $\Phi^\times$.

By using prescription (35), we can also define for each eigenvalue p the eigenbra $\langle p|$ associated with the eigenfunction (23):

$$\langle p|\varphi\rangle \equiv \int_{-\infty}^{\infty} dx\, \varphi(x)\frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar} \equiv \int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|\varphi\rangle\,. \tag{44}$$

Comparison with Eq. (38) shows that the action of $\langle p|$ is the complex conjugate of the action of $|p\rangle$,

$$\langle p|\varphi\rangle = \overline{\langle\varphi|p\rangle}\,, \tag{45}$$

and that

$$\langle p|x\rangle = \overline{\langle x|p\rangle} = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}\,. \tag{46}$$

The bra $\langle x|$ is defined as

$$\langle x|\varphi\rangle \equiv \int_{-\infty}^{\infty} dx'\, \varphi(x')\delta(x-x') \equiv \int_{-\infty}^{\infty} dx'\, \langle x|x'\rangle\langle x'|\varphi\rangle\,. \tag{47}$$

Comparison with Eq. (40) shows that the action of $\langle x|$ is complex conjugated to the action of $|x\rangle$,

$$\langle x|\varphi\rangle = \overline{\langle\varphi|x\rangle}\,, \tag{48}$$

and that

$$\langle x|x'\rangle = \langle x'|x\rangle = \delta(x-x')\,. \tag{49}$$

Analogously, the eigenbras of the Hamiltonian are defined as

$${}_{\text{l,r}}\langle^+E|\varphi\rangle \equiv \int_{-\infty}^{\infty} dx\, \varphi(x)\, {}_{\text{l,r}}\langle^+E|x\rangle \equiv \int_{-\infty}^{\infty} dx\, {}_{\text{l,r}}\langle^+E|x\rangle\langle x|\varphi\rangle\,, \tag{50}$$

where

$${}_{\text{l,r}}\langle^+E|x\rangle = \overline{\langle x|E^+\rangle}_{\text{l,r}}\,. \tag{51}$$

Comparison of Eq. (50) with Eq. (42) shows that the actions of the bras ${}_{\text{l,r}}\langle^+E|$ are the complex conjugates of the actions of the kets $|E^+\rangle_{\text{l,r}}$:

$${}_{\text{l,r}}\langle^+E|\varphi\rangle = \overline{\langle\varphi|E^+\rangle}_{\text{l,r}}\,. \tag{52}$$

Now, by using the rigged Hilbert space, one can show that the definitions of $\langle p|$, $\langle x|$ and ${}_{\text{l,r}}\langle^+E|$ make sense and that $\langle p|$, $\langle x|$ and ${}_{\text{l,r}}\langle^+E|$ belong to Φ'.

It is important to keep in mind the difference between eigenfunctions and kets. For instance, $\langle x|p\rangle$ is an eigenfunction of a differential equation, Eq. (20), whereas $|p\rangle$ is a functional, the relation between them being given by Eq. (39). A similar relation holds between $\langle x'|x\rangle$ and $|x\rangle$, and between $\langle x|E^+\rangle_{\mathrm{l,r}}$ and $|E^+\rangle_{\mathrm{l,r}}$. It is also important to keep in mind that "scalar products" like $\langle x|p\rangle$, $\langle x'|x\rangle$ or $\langle x|E^+\rangle_{\mathrm{l,r}}$ do not represent an actual scalar product of two functionals; these "scalar products" are simply solutions to differential equations.

The kets $|p\rangle$, $|x\rangle$ and $|E^+\rangle_{\mathrm{l,r}}$ are indeed eigenvectors of P, Q and H, respectively:

$$P|p\rangle = p|p\rangle \, , \quad p \in \mathbb{R} \, , \tag{53}$$

$$Q|x\rangle = x|x\rangle \, , \quad x \in \mathbb{R} \, , \tag{54}$$

$$H|E^+\rangle_{\mathrm{l,r}} = E|E^+\rangle_{\mathrm{l,r}} \, , \quad E \in [0,\infty) \, . \tag{55}$$

Similarly, the bras $\langle p|$, $\langle x|$ and ${}_{\mathrm{l,r}}\langle {}^+E|$ are left eigenvectors of P, Q and H, respectively:

$$\langle p|P = p\langle p| \, , \quad p \in \mathbb{R} \, , \tag{56}$$

$$\langle x|Q = x\langle x| \, , \quad x \in \mathbb{R} \, , \tag{57}$$

$${}_{\mathrm{l,r}}\langle {}^+E|H = E \; {}_{\mathrm{l,r}}\langle {}^+E| \, , \quad E \in [0,\infty) \, . \tag{58}$$

Note that these equations are to be understood in the distributional way, that is, as "sandwiches" with elements of Φ. For example, Eq. (53) should be understood as

$$\langle \varphi|P|p\rangle = p\langle \varphi|p\rangle \, , \quad p \in \mathbb{R} \, , \; \varphi \in \Phi \, , \tag{59}$$

and the same for (54)-(58). Usually, the "sandwiching" is implicit and therefore omitted.

Now that we have constructed the Dirac bras and kets, we can see how other aspects of Dirac's bra-ket formalism hold within the rigged Hilbert space. For example, the completeness relations

$$\int_{-\infty}^{\infty} dp \, |p\rangle\langle p| = I \, , \tag{60}$$

$$\int_{-\infty}^{\infty} dx' \, |x'\rangle\langle x'| = I \, , \tag{61}$$

$$\int_0^{\infty} dE \, |E^+\rangle_{\mathrm{l\,l}}\langle {}^+E| + \int_0^{\infty} dE \, |E^+\rangle_{\mathrm{r\,r}}\langle {}^+E| = I \, , \tag{62}$$

and the action of P, Q and H,

$$P = \int_{-\infty}^{\infty} dp \, p|p\rangle\langle p| \, , \tag{63}$$

$$Q = \int_{-\infty}^{\infty} dx x|x\rangle\langle x| \, , \tag{64}$$

$$H = \int_0^{\infty} dE \, E|E^+\rangle_{\mathrm{l\,l}}\langle {}^+E| + \int_0^{\infty} dE \, E|E^+\rangle_{\mathrm{r\,r}}\langle {}^+E| \, , \tag{65}$$

all hold within the rigged Hilbert space as a "sandwich" with elements of Φ. Other expressions such as the delta normalization of eigenfunctions, e.g.,

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\, e^{i(p-p')x/\hbar} = \delta(p-p')\,, \tag{66}$$

or the "matrix elements" of the observables, e.g.,

$$\langle x|Q|x'\rangle = x'\,\delta(x-x')\,, \tag{67}$$

$$\langle x|P|x'\rangle = -i\hbar\frac{d}{dx}\,\delta(x-x')\,, \tag{68}$$

$$\langle x|H|x'\rangle = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\delta(x-x')\,. \tag{69}$$

are interpreted the same way.

To conclude this section, I would like to refer the reader to [5, 6] for a detailed account of the above results.

THE RIGGED HILBERT SPACE OF THE LIPPMANN-SCHWINGER EQUATION: LECTURE 3

The Lippmann-Schwinger equation is one of the cornerstones of scattering theory. It is written as

$$|E^{\pm}\rangle = |E\rangle + \frac{1}{E-H_0\pm i\varepsilon}V|E^{\pm}\rangle\,, \tag{70}$$

where $|E^{\pm}\rangle$ are the "in" and "out" Lippmann-Schwinger kets, $|E\rangle$ is an eigenket of the free Hamiltonian H_0,

$$H_0|E\rangle = E|E\rangle\,, \tag{71}$$

and V is the potential. The Lippmann-Schwinger kets are, in particular, eigenvectors of H:

$$H|E^{\pm}\rangle = E|E^{\pm}\rangle\,. \tag{72}$$

To the kets $|E^{\pm}\rangle$, there correspond the bras $\langle^{\pm}E|$, which satisfy

$$\langle^{\pm}E| = \langle E| + \langle^{\pm}E|V\frac{1}{E-H_0\mp i\varepsilon}\,. \tag{73}$$

The bras $\langle^{\pm}E|$ are left eigenvectors of H,

$$\langle^{\pm}E|H = E\langle^{\pm}E|\,, \tag{74}$$

and the bras $\langle E|$ are left eigenvectors of H_0,

$$\langle E|H_0 = E\langle E|\,. \tag{75}$$

The Lippmann-Schwinger equation (70) for the "in" $|E^+\rangle$ and "out" $|E^-\rangle$ kets has the scattering "in" and "out" boundary conditions built into the $\pm i\varepsilon$, since Eq. (70) is equivalent to the time-independent Schrödinger equation (72) subject to those "in" ($+i\varepsilon$) and "out" ($-i\varepsilon$) boundary conditions. In the position representation, the $\pm i\varepsilon$ prescriptions yield the following asymptotic behaviors:

$$\langle \mathbf{x}|E^+\rangle \xrightarrow[r\to\infty]{} e^{ikz} + f(k,\theta)\frac{e^{ikr}}{r}\,, \tag{76}$$

$$\langle \mathbf{x}|E^-\rangle \xrightarrow[r\to\infty]{} e^{ikz} + \overline{f(k,\theta)}\frac{e^{-ikr}}{r}\,, \tag{77}$$

where $\mathbf{x} \equiv (x,y,z) \equiv (r,\theta,\phi)$ are the position coordinates, k is the wave number of Eq. (26) and $f(k,\theta)$ is the scattering amplitude.

Likewise any bra and ket, the Lippmann-Schwinger bras and kets do not have a place in the Hilbert space. In this lecture, we will construct the rigged Hilbert space to which they belong. We will use the example of the spherical shell potential.

The radial Lippmann-Schwinger equation

For the spherical shell potential,

$$V(\mathbf{x}) \equiv V(r) = \begin{cases} 0 & 0<r<a \\ V_0 & a<r<b \\ 0 & b<r<\infty\,, \end{cases} \tag{78}$$

the Lippmann-Schwinger equation can be solved explicitly. Because the potential (78) is spherically symmetric, we will work in the radial position representation and restrict ourselves to angular momentum $l=0$.

In the radial representation, the Lippmann-Schwinger equation (70) becomes

$$\langle r|E^\pm\rangle = \langle r|E\rangle + \langle r|\frac{1}{E-H_0 \pm i\varepsilon}V|E^\pm\rangle\,. \tag{79}$$

The procedure to solve Eq. (79) is well known. Since Eq. (79) is an integral equation, it is equivalent to a differential equation subject to the boundary conditions that are built into it. In our case, for $l=0$, Eq. (79) is equivalent to the Schrödinger differential equation,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)\langle r|E^\pm\rangle = E\langle r|E^\pm\rangle\,, \tag{80}$$

subject to the following boundary conditions:

$$\langle r|E^\pm\rangle = 0\,, \tag{81}$$

$$\langle r|E^\pm\rangle \text{ is continuous at } r=a,b\,, \tag{82}$$

$$\frac{d}{dr}\langle r|E^\pm\rangle \text{ is continuous at } r=a,b\,, \tag{83}$$

$$\langle r|E^+\rangle \sim e^{-ikr} - S(E)\, e^{ikr} \quad \text{as } r\to\infty\,, \tag{84}$$
$$\langle r|E^-\rangle \sim e^{ikr} - \overline{S(E)}\, e^{-ikr} \quad \text{as } r\to\infty\,, \tag{85}$$

where $S(E)$ is the S matrix in the energy representation. The boundary conditions (84) and (85) originate from the $\pm i\varepsilon$ conditions of Eq. (79). The asymptotic behaviors (84) and (85) are the $l=0$, radial counterparts of the asymptotic behaviors (76) and (77).

If we insert (78) into (80), and solve (80) subject to (81)-(85), we obtain

$$\langle r|E^\pm\rangle \equiv \chi^\pm(r;E) = N(E)\,\frac{\chi(r;E)}{\mathscr{J}_\pm(E)}\,, \qquad E\in[0,\infty)\,, \tag{86}$$

where $N(E)$ is a delta-normalization factor,

$$N(E) = \sqrt{\frac{1}{\pi}\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}}\,, \tag{87}$$

$\chi(r;E)$ is the so-called regular solution of Eq. (80),

$$\chi(r;E) = \begin{cases} \sin(\sqrt{\frac{2m}{\hbar^2}E}\,r) & 0<r<a \\ \mathscr{J}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}\,r} + \mathscr{J}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}\,r} & a<r<b \\ \mathscr{J}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}\,r} + \mathscr{J}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}\,r} & b<r<\infty\,, \end{cases} \tag{88}$$

and $\mathscr{J}_\pm(E)$ are the Jost functions,

$$\mathscr{J}_+(E) = -2i\mathscr{J}_4(E)\,, \tag{89}$$

$$\mathscr{J}_-(E) = 2i\mathscr{J}_3(E)\,. \tag{90}$$

The explicit expressions for $\mathscr{J}_1$-$\mathscr{J}_4$ can be obtained by matching the values of $\chi(r;E)$ and of its derivative at the discontinuities of the potential. In terms of the Jost functions, the S matrix is given by

$$S(E) = \frac{\mathscr{J}_-(E)}{\mathscr{J}_+(E)}\,, \qquad E\in[0,\infty)\,. \tag{91}$$

Similarly to the "right" ones, we can obtain the "left" Lippmann-Schwinger eigenfunctions by writing Eq. (73) in the radial position representation,

$$\langle^\pm E|r\rangle = \langle E|r\rangle + \langle^\pm E|V\frac{1}{E-H_0\mp i\varepsilon}|r\rangle\,. \tag{92}$$

Solving Eq. (92) is analogous to solving Eq. (79). The solutions to (92) are the complex conjugates of the solutions to (79):

$$\langle^\pm E|r\rangle = \overline{\chi^\pm(r;E)} = \chi^\mp(r;E)\,. \tag{93}$$

The rigged Hilbert space of the Lippmann-Schwinger bras and kets

By using (34), we associate "in" and "out" kets $|E^{\pm}\rangle$ with the eigenfunctions $\chi^{\pm}(r;E)$ for each $E \in [0,\infty)$:

$$\langle \varphi^{\pm}|E^{\pm}\rangle \equiv \int_0^{\infty} dr\, \overline{\varphi^{\pm}(r)}\chi^{\pm}(r;E) \equiv \int_0^{\infty} dr\, \langle \varphi^{\pm}|r\rangle\langle r|E^{\pm}\rangle \,, \tag{94}$$

where $\varphi^{\pm}$ belong to the space Φ that will be constructed below. (Note that the Φ of this lecture is different from the Φ of Lecture 2.) Similarly, by using (35), we define the bras $\langle^{\pm}E|$ as

$$\langle^{\pm}E|\varphi^{\pm}\rangle \equiv \int_0^{\infty} dr\, \overline{\chi^{\pm}(r;E)}\varphi^{\pm}(r) \equiv \int_0^{\infty} dr\, \langle^{\pm}E|r\rangle\langle r|\varphi^{\pm}\rangle \,. \tag{95}$$

Note that even though $\chi^{\pm}(r;E) \equiv \langle r|E^{\pm}\rangle$ are also meaningful for complex energies, the energy in Eqs. (94) and (95) runs only over $\mathrm{Sp}(H) = [0,\infty)$, because in this lecture we restrict ourselves to bras and kets associated with energies that belong to the scattering spectrum of the Hamiltonian.

From definitions (94) and (95), it follows that the action of $\langle^{\pm}E|$ is complex conjugated to the action of $|E^{\pm}\rangle$:

$$\langle^{\pm}E|\varphi^{\pm}\rangle = \overline{\langle \varphi^{\pm}|E^{\pm}\rangle} \,. \tag{96}$$

We now need to find the subspace Φ on which the above definitions make sense. Besides making (94)-(95) well defined, the space Φ must also be invariant under the action of the observables of the system. Since in this lecture the only observable we are concerned with is the Hamiltonian, we will simply require invariance under H. Thus, the space Φ must satisfy the following conditions:

- The space Φ is invariant under the action of H. (97)
- The elements of Φ are such that the integrals in Eqs. (94)–(95) make sense. (98)

In order to meet requirement (97), the wave functions $\varphi^{\pm}(r)$ must at least be in the maximal invariant subspace of H:

$$\mathscr{D} = \bigcap_{n=0}^{\infty} \mathscr{D}(H^n) \,. \tag{99}$$

In order to meet requirement (98), the wave functions $\varphi^{\pm}(r)$ must behave well enough so the integrals in Eqs. (94)-(95) are well defined. From the expression for $\chi^{\pm}(r;E)$, Eq. (86), one can see that the $\varphi^{\pm}(r)$ have essentially to control purely imaginary exponentials. Therefore, the space Φ that meets the requirements (97)-(98) is

$$\Phi = \left\{ \varphi^{\pm} \in L^2([0,\infty),dr) \mid \varphi^{\pm} \in \mathscr{D} \,,\ \|\varphi^{\pm}\|_{n,m} < \infty \,,\ n,m = 0,1,2,\ldots \right\} , \tag{100}$$

where the $\|\ \|_{n,m}$ are given by

$$\|\varphi^{\pm}\|_{n,m} = \sqrt{\int_0^{\infty} dr\, |(1+r)^n(1+H)^m\varphi^{\pm}(r)|^2} \,, \quad n,m = 0,1,2,\ldots \,. \tag{101}$$

The space Φ is thus the collection of square integrable functions that belong to the maximal invariant subspace of H and for which the estimates (101) are finite. In particular, because $\varphi^{\pm}(r)$ satisfy the estimates (101), $\varphi^{\pm}(r)$ fall off at infinity faster than any polynomial of r:

$$\lim_{r\to\infty}(1+r)^n\varphi^{\pm}(r)=0\,,\quad n=0,1,2,\ldots\,. \tag{102}$$

Thus, likewise in Lecture 2, we have obtained a Schwartz-like space. Obviously, the space Φ can also be seen as the maximal invariant subspace of the algebra generated by the Hamiltonian and the operator multiplication by r.

Note that we have used superscripts $\pm$ to denote the elements of one and the same space Φ. The reason is that when we use $+$, it means that the elements of Φ are acted upon by $|E^+\rangle$ or $\langle^+E|$, and when we use $-$, they are acted upon by $|E^-\rangle$ or $\langle^-E|$.

We can now construct the spaces Φ' and $\Phi^{\times}$, and see that $|E^{\pm}\rangle$ belong to $\Phi^{\times}$, whereas $\langle^{\pm}E|$ belong to Φ'. Thus, the Lippmann-Schwinger equations (70) and (73), Eqs. (72) and (74), as well as

$$e^{-iHt/\hbar}|E^{\pm}\rangle=e^{-iEt/\hbar}|E^{\pm}\rangle\,, \tag{103}$$

$$\langle^{\pm}E|e^{-iHt/\hbar}=e^{iEt/\hbar}\langle^{\pm}E|\,, \tag{104}$$

hold in the distributional sense, i.e., as "sandwiches" with elements of Φ.

For a detailed account on the results of this lecture, the reader may wish to refer to [7].

THE RIGGED HILBERT SPACE OF THE ANALYTIC CONTINUATION OF THE THE LIPPMANN-SCHWINGER EQUATION: LECTURE 4

This lecture is devoted to construct and characterize the analytic continuation of the Lippmann-Schwinger bras and kets. As in Lecture 3, we restrict ourselves to the spherical shell potential (78) and zero angular momentum.

The ultimate goal we want to achieve by analytically continuing the solutions of the Lippmann-Schwinger equation is to obtain, in Lecture 5, the resonance (decay) amplitude.

The wave number representation

The Lippmann-Schwinger eigenfunctions depend explicitly on the wave number k of Eq. (26) rather than on the energy E. It is therefore convenient to rewrite their expressions in terms of k before performing analytic continuations.

We start by writing the regular solution (88) in terms of k:

$$\chi(r;k)=\chi(r;E)=\begin{cases}\sin(kr) & 0<r<a\\ \mathcal{J}_1(k)e^{i\kappa r}+\mathcal{J}_2(k)e^{-i\kappa r} & a<r<b\\ \mathcal{J}_3(k)e^{ikr}+\mathcal{J}_4(k)e^{-ikr} & b<r<\infty\,,\end{cases} \tag{105}$$

where κ is given by (26). In terms of k, the Lippmann-Schwinger eigenfunctions read as

$$\chi^{\pm}(r;E) = \sqrt{\frac{1}{\pi}\frac{2m/\hbar^2}{k}}\,\frac{\chi(r;k)}{\mathscr{J}_{\pm}(k)}\,. \tag{106}$$

The eigenfunctions $\chi^{\pm}(r;E)$ are δ-normalized as functions of E. The Lippmann-Schwinger eigenfunctions that are δ-normalized as functions of k are given by

$$\chi^{\pm}(r;k) \equiv \sqrt{\frac{\hbar^2}{2m}2k}\,\chi^{\pm}(r;E) = \sqrt{\frac{2}{\pi}}\,\frac{\chi(r;k)}{\mathscr{J}_{\pm}(k)}\,. \tag{107}$$

In bra-ket notation, we will write

$$\langle r|k^{\pm}\rangle = \chi^{\pm}(r;k)\,, \quad k>0\,, \tag{108}$$

$$\langle^{\pm}k|r\rangle = \overline{\chi^{\pm}(r;k)} = \chi^{\mp}(r;k)\,, \quad k>0\,. \tag{109}$$

Because of (107), in terms of k the Lippmann-Schwinger bras and kets read as

$$\langle^{\pm}k| = \sqrt{\frac{\hbar^2}{2m}2k}\,\langle^{\pm}E|\,, \quad k>0\,, \tag{110}$$

$$|k^{\pm}\rangle = \sqrt{\frac{\hbar^2}{2m}2k}\,|E^{\pm}\rangle\,, \quad k>0\,. \tag{111}$$

The bras $\langle^{\pm}k|$ and kets $|k^{\pm}\rangle$ are, respectively, left and right eigenvectors of H with eigenvalue $\frac{\hbar^2}{2m}k^2$:

$$\langle^{\pm}k|H = \frac{\hbar^2}{2m}k^2\langle^{\pm}k|\,, \tag{112}$$

$$H|k^{\pm}\rangle = \frac{\hbar^2}{2m}k^2|k^{\pm}\rangle\,. \tag{113}$$

The analytic continuation of the Lippmann-Schwinger eigenfunctions

The analytic continuation of $\chi^{\pm}(r;k)$ is done as follows. First, one specifies the boundary values that the Lippmann-Schwinger eigenfunctions take on the positive k-axis. And second, one continues those boundary values into the whole k-plane. Since the boundary values of the Lippmann-Schwinger eigenfunctions on the positive k-axis are given by Eq. (107), and since $\chi^{\pm}(r;k)$ are expressed in terms of well-known analytic functions, the continuation of $\chi^{\pm}(r;k)$ from the positive k-axis into the whole wave-number plane is well defined.

A word on notation. Whenever they become complex, we will denote the energy E and the wave number k by respectively z and q. Accordingly, the continuations of

$\chi^{\pm}(r;E)$ and $\chi^{\pm}(r;k)$ will be denoted by $\chi^{\pm}(r;z)$ and $\chi^{\pm}(r;q)$. In bra-ket notation, the analytically continued eigenfunctions will be written as

$$\langle r|q^{\pm}\rangle = \chi^{\pm}(r;q)\,, \tag{114}$$

$$\langle^{\pm}q|r\rangle = \chi^{\mp}(r;q)\,. \tag{115}$$

Note that, in distinction to (93), the analytically continued "left" eigenfunction is not the complex conjugate of the "right" eigenfunction but

$$\langle^{\pm}q|r\rangle = \overline{\langle r|\overline{q}^{\pm}\rangle}\,. \tag{116}$$

In order to characterize the analytic properties of $\chi^{\pm}(r;q)$, it is useful to define

$$Z_{\pm} \equiv \{q \in \mathbb{C} \mid \mathscr{J}_{\pm}(q) = 0\}\,. \tag{117}$$

The elements of Z_{+} are simply the resonance energies. Since $\chi(r;q)$ and $\mathscr{J}_{\pm}(q)$ are analytic in the whole k-plane, $\chi^{\pm}(r;q)$ is analytic in the whole k-plane except at $Z_{\pm}$, where its poles are located.

In order to define the analytically continued Lippmann-Schwinger bras and kets, we need to know how $\chi^{\pm}(r;q)$ grow with q. To find out, let us recall first that the growth of $\chi(r;q)$ is bounded by [8]

$$|\chi(r;q)| \leq C\,\frac{|q|\,r}{1+|q|\,r}\,e^{|\mathrm{Im}(q)|r}\,, \quad q \in \mathbb{C}\,. \tag{118}$$

From Eqs. (107) and (118), it follows that the eigenfunctions $\chi^{\pm}(r;q)$ satisfy

$$\left|\chi^{\pm}(r;q)\right| \leq \frac{C}{|\mathscr{J}_{\pm}(q)|}\,\frac{|q|r}{1+|q|r}\,e^{|\mathrm{Im}(q)|r}\,. \tag{119}$$

When $q \in Z_{\pm}$, $\chi^{\pm}(r;q)$ blows up to infinity.

We can further refine the estimates (119) by characterizing the growth of $1/|\mathscr{J}_{\pm}(q)|$ in different regions of the complex plane. In the upper half of the complex k-plane, the inverse of $\mathscr{J}_{+}(q)$ is bounded:

$$\frac{1}{|\mathscr{J}_{+}(q)|} \leq C\,, \quad \mathrm{Im}(q) \geq 0\,. \tag{120}$$

In the lower half-plane, $\frac{1}{\mathscr{J}_{+}(q)}$ is infinite whenever $q \in Z_{+}$. As $|q|$ tends to ∞ in the lower half plane, we have

$$\frac{1}{\mathscr{J}_{+}(q)} \approx \frac{1}{1-Cq^{-2}e^{2iqb}}\,, \quad (|q| \to \infty,\ \mathrm{Im}(q) < 0)\,. \tag{121}$$

The above estimates are satisfied by $\mathscr{J}_{-}(q)$ when we exchange the upper for the lower half plane, and Z_{+} for Z_{-}.

The analytic continuation of the Lippmann-Schwinger bras and kets

The analytic continuation of the Lippmann-Schwinger bras is defined for any complex wave number q in the distributional way (35):

$$\langle {}^{\pm}q|\varphi^{\pm}\rangle \equiv \int_0^{\infty} dr\, \varphi^{\pm}(r)\chi^{\mp}(r;q) = \int_0^{\infty} dr\, \langle {}^{\pm}q|r\rangle\langle r|\varphi^{\pm}\rangle\,, \tag{122}$$

where the functions $\varphi^{\pm}(r)$ belong to a space of test functions $\Phi_{\rm exp}$ that will be constructed below. Similarly to the bras, the analytic continuation of the Lippmann-Schwinger kets is defined by way of (34):

$$\langle \varphi^{\pm}|q^{\pm}\rangle \equiv \int_0^{\infty} dr\, \overline{\varphi^{\pm}(r)}\chi^{\pm}(r;q) = \int_0^{\infty} dr\, \langle \varphi^{\pm}|r\rangle\langle r|q^{\pm}\rangle\,. \tag{123}$$

Note that definition (122) is actually a slight generalization of (35), due to (116).

The bras (122) and kets (123) are defined for all complex q except at those q at which the corresponding eigenfunction has a pole. At those poles, one can still define bras and kets if in definitions (122) and (123) one substitutes the eigenfunctions $\chi^{\pm}(r;q)$ by their residues at the pole.

From the analytic continuation of the bras and kets into any complex wave number, one can now obtain the analytic continuation of the bras and kets into any complex energy of the Riemann surface (compare with Eqs. (110) and (111)):

$$|z^{\pm}\rangle = \sqrt{\frac{2m}{\hbar^2}\frac{1}{2q}}\,|q^{\pm}\rangle\,, \quad \langle {}^{\pm}z| = \sqrt{\frac{2m}{\hbar^2}\frac{1}{2q}}\,\langle {}^{\pm}q|\,. \tag{124}$$

Construction of the rigged Hilbert space

Likewise the bras and kets associated with real energies, the analytic continuation of the Lippmann-Schwinger bras and kets must be described within the rigged Hilbert space rather than just within the Hilbert space. We will denote the rigged Hilbert space for the analytically continued bras by

$$\Phi_{\rm exp} \subset L^2([0,\infty),dr) \subset \Phi'_{\rm exp}\,, \tag{125}$$

and the one for the analytically continued kets by

$$\Phi_{\rm exp} \subset L^2([0,\infty),dr) \subset \Phi^{\times}_{\rm exp}\,. \tag{126}$$

The functions $\varphi^{\pm} \in \Phi_{\rm exp}$ must satisfy the following conditions:

- They belong to the maximal invariant subspace $\mathscr{D}$ of H, see Eq. (99). (127)

- They are such that definitions (122) and (123) make sense. (128)

The reason why $\varphi^{\pm}$ must satisfy condition (127) is that such condition guarantees that all the powers of the Hamiltonian are well defined. Condition (127), however, is not sufficient to obtain well-defined bras and kets associated with complex wave numbers. In order for $\langle^{\pm}q|$ and $|q^{\pm}\rangle$ to be well defined, the wave functions $\varphi^{\pm}(r)$ must be well behaved so the integrals in Eqs. (122) and (123) converge. Since by Eq. (119) $\chi^{\pm}(r;q)$ grow exponentially with r, the wave functions $\varphi^{\pm}(r)$ have to, essentially, tame real exponentials. If we define

$$\|\varphi^{\pm}\|_{n,n'} \equiv \sqrt{\int_0^{\infty} dr \left| \frac{nr}{1+nr} e^{nr^2/2}(1+H)^{n'}\varphi^{\pm}(r)\right|^2} \, , \quad n,n'=0,1,2,\ldots \, , \qquad (129)$$

then the space $\Phi_{\rm exp}$ is given by

$$\Phi_{\rm exp} = \left\{ \varphi^{\pm} \in \mathscr{D} \,|\, \|\varphi^{\pm}\|_{n,n'} < \infty \, , \; n,n'=0,1,2,\ldots \right\} . \qquad (130)$$

This is just the space of square integrable functions which belong to the maximal invariant subspace of H and for which the quantities (129) are finite. In particular, because $\varphi^{\pm}(r)$ satisfy the estimates (129), their tails fall off faster than Gaussians.

From Eq. (119), it is clear that the integrals in Eqs. (122) and (123) converge already for functions that fall off at infinity faster than any exponential. We have imposed Gaussian falloff because it will allow us to perform resonance expansions in Lecture 5.

It is illuminating to compare the space Φ of Lecture 3 with the space $\Phi_{\rm exp}$ of Eq. (130). Because for real wave numbers the Lippmann-Schwinger eigenfunctions behave like purely imaginary exponentials, in Lecture 3 we only needed to impose on the test functions a polynomial falloff, thereby obtaining a space of test functions very similar to the Schwartz space. By contrast, for complex wave numbers the Lippmann-Schwinger eigenfunctions blow up exponentially, and therefore we need to impose on the test functions an exponential falloff that damps such an exponential blowup.

One can now easily show that the kets $|q^{\pm}\rangle$ belong to $\Phi_{\rm exp}^{\times}$ and satisfy

$$H|q^{\pm}\rangle = \frac{\hbar^2}{2m}q^2\,|q^{\pm}\rangle \, , \qquad (131)$$

$$e^{-iHt/\hbar}|q^{\pm}\rangle = e^{-iq^2\hbar t/(2m)}|q^{\pm}\rangle \, . \qquad (132)$$

Similarly, $\langle^{\pm}q| \in \Phi_{\rm exp}'$ and

$$\langle^{\pm}q|H = \frac{\hbar^2}{2m}q^2\langle^{\pm}q| \, , \qquad (133)$$

$$\langle^{\pm}q|e^{-iHt/\hbar} = e^{iq^2\hbar t/(2m)}\langle^{\pm}q| \, . \qquad (134)$$

Equations (131) and (133) can be rewritten in terms of the complex energy z as

$$H|z^{\pm}\rangle = z|z^{\pm}\rangle \, , \qquad (135)$$

$$\langle^{\pm}z|H = z\langle^{\pm}z| \, . \qquad (136)$$

Note that (136) is not given by $\langle^{\pm}z|H = \overline{z}\langle^{\pm}z|$, as one may naively expect from formally obtaining (136) by Hermitian conjugation of (135).

For a full account of this lecture, the reader can refer to [9].

RESONANCE STATES, AND THEIR RIGGED HILBERT SPACE: LECTURE 5

The Gamow states are the state vectors of resonances. They are eigenvectors of the Hamiltonian with a complex eigenvalue. The real (imaginary) part of the complex eigenvalue is associated with the energy (width) of the resonance.

Because self-adjoint operators on a Hilbert space can only have real eigenvalues, the Gamow states fit not within the Hilbert space but within the rigged Hilbert space. In this lecture, we will see that the Gamow states belong to the rigged Hilbert space of Lecture 4.

Like in Lectures 3 and 4, we will use the spherical shell potential (78) and study the zero angular momentum case only. Unlike in Lecture 4, we will write most results in terms of the energy, because they tend to be simpler than in terms of the wave number. The energy and the wave number of a resonance R will be denoted by $z_{\rm R}$ and $k_{\rm R}$.

The Gamow eigenfunctions satisfy the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)u(r;z_{\rm R})=z_{\rm R}\,u(r;z_{\rm R})\,, \tag{137}$$

subject to "purely outgoing boundary conditions,"

$$u(0;z_{\rm R})=0\,, \tag{138}$$

$$u(r;z_{\rm R}) \text{ is continuous at } r=a,b\,, \tag{139}$$

$$\frac{d}{dr}u(r;z_{\rm R}) \text{ is continuous at } r=a,b\,, \tag{140}$$

$$u(r;z_{\rm R})\sim e^{ik_{\rm R}r} \text{ as } r\to\infty\,, \tag{141}$$

where (141) is the "purely outgoing boundary condition" (POBC). Comparison of (138)-(141) with (81)-(85) shows that it is the POBC what selects the resonance energies.

For the potential (78), the only possible eigenvalues of (137) subject to (138)-(141) are the zeros of the Jost function,

$$\mathscr{J}_+(z_{\rm R})=0\,. \tag{142}$$

The solutions of this equation come as a denumerable number of complex conjugate pairs z_n, z_n^*. The number $z_n=E_n-i\Gamma_n/2$ is the nth resonance energy, and $z_n^*=E_n+i\Gamma_n/2$ is the nth anti-resonance energy. The corresponding wave numbers are

$$k_n=\sqrt{\frac{2m}{\hbar^2}z_n}\,,\quad -k_n^*=\sqrt{\frac{2m}{\hbar^2}z_n^*}\,,\quad n=1,2,\ldots\,. \tag{143}$$

For the potential (78), the resonance energies are simple poles of the S matrix (see [10] for an example of a potential that produces double poles). In order to write expressions for resonances and anti-resonances together, we will label the resonances by a positive integer $n=1,2,\ldots$ and the anti-resonances by a negative integer $n=-1,-2,\ldots$.

The nth Gamow eigensolution, $n = \pm 1, \pm 2, \ldots$, reads

$$u(r;z_n) = u(r;k_n) = N_n \begin{cases} \frac{1}{\mathscr{J}_3(k_n)} \sin(k_n r) & 0 < r < a \\ \frac{\mathscr{J}_1(k_n)}{\mathscr{J}_3(k_n)} e^{iQ_n r} + \frac{\mathscr{J}_2(k_n)}{\mathscr{J}_3(k_n)} e^{-iQ_n r} & a < r < b \\ e^{ik_n r} & b < r < \infty \, , \end{cases} \tag{144}$$

where

$$Q_n = \sqrt{\frac{2m}{\hbar^2}(z_n - V_0)} \, , \tag{145}$$

and N_n is a normalization factor,

$$N_n^2 = i \, \mathrm{res} \left[S(q) \right]_{q=k_n} \, . \tag{146}$$

The Gamow eigenfunctions (144) are related with $\chi^{\pm}(r;q)$ by

$$u(r;k_n) = -\frac{\sqrt{2\pi}}{N_n} \mathrm{res} \left[\chi^+(r;q) \right]_{q=k_n} \, , \tag{147}$$

$$u(r;k_n) = i\sqrt{2\pi} N_n \chi^-(r;k_n) \, . \tag{148}$$

Because of (148) and (116), the "left" Gamow eigenfunctions read

$$\langle z_n | r \rangle = [u(r;z_n^*)]^* \, , \quad n = \pm 1, \pm 2, \ldots \, . \tag{149}$$

Thus, the "left" Gamow eigenfunction is not just the complex conjugate of the "right" eigenfunction, but the complex conjugated eigenfunction evaluated at the complex conjugated energy. Because the Gamow eigenfunctions satisfy

$$[u(r;z_n^*)]^* = u(r;z_n) \, , \quad n = \pm 1, \pm 2, \ldots \, , \tag{150}$$

the "left" and the "right" Gamow eigenfunctions are actually the same eigenfunction,

$$\langle z_n | r \rangle = [u(r;z_n^*)]^* = u(r;z_n) = \langle r | z_n \rangle \, , \quad n = \pm 1, \pm 2, \ldots \, . \tag{151}$$

In terms of the wave number, Eq. (151) reads as

$$\langle k_n | r \rangle = [u(r;-k_n^*)]^* = u(r;k_n) = \langle r | k_n \rangle \, , \quad n = \pm 1, \pm 2, \ldots \, . \tag{152}$$

The Gamow eigenfunctions $u(r;z_n)$ are not square integrable and therefore must be treated as distributions. By treating them as distributions, we will be able to generate the Gamow bras and kets. According to (34), the Gamow ket $|z_n\rangle$ associated with the eigenfunction $u(r;z_n)$ must be defined as

$$\langle \varphi | z_n \rangle \equiv \int_0^{\infty} dr \, [\varphi(r)]^* \, u(r;z_n) = \int_0^{\infty} dr \, \langle \varphi | r \rangle \langle r | z_n \rangle \, , \quad n = \pm 1, \pm 2, \ldots \, . \tag{153}$$

Similarly, the Gamow bra associated with the resonance (or anti-resonance) energy z_n is defined as

$$\langle z_n|\varphi\rangle \equiv \int_0^\infty dr\, \varphi(r)u(r;z_n) = \int_0^\infty dr\, \langle z_n|r\rangle\langle r|\varphi\rangle\,, \quad n = \pm 1, \pm 2, \ldots\,. \tag{154}$$

From these definitions and from Eqs. (147) and (148), it is clear that the Gamow bras and kets are accommodated by the rigged Hilbert spaces (125) and (126).

Within the rigged Hilbert spaces (125) and (126), it holds that the Gamow bras and kets are eigenvectors of the Hamiltonian:

$$H|z_n\rangle = z_n\,|z_n\rangle\,, \quad n = \pm 1, \pm 2, \ldots\,, \tag{155}$$

$$\langle z_n|H = z_n\langle z_n|\,, \quad n = \pm 1, \pm 2, \ldots\,. \tag{156}$$

Because their energy is complex, the time evolution of the Gamow bras and kets should be time asymmetric. For resonances, it should be that

$$\langle z_n|e^{-iHt/\hbar} = e^{iz_nt/\hbar}\langle z_n|\,, \quad \text{only for } t < 0\,,\ n = 1, 2, \ldots\,, \tag{157}$$

$$e^{-iHt/\hbar}|z_n\rangle = e^{-iz_nt/\hbar}|z_n\rangle\,, \quad \text{only for } t > 0\,,\ n = 1, 2, \ldots\,, \tag{158}$$

whereas for anti-resonances, it should be that

$$\langle z_n|e^{-iHt/\hbar} = e^{iz_nt/\hbar}\langle z_n|\,, \quad \text{only for } t > 0\,,\ n = -1, -2, \ldots\,, \tag{159}$$

$$e^{-iHt/\hbar}|z_n\rangle = e^{-iz_nt/\hbar}|z_n\rangle\,, \quad \text{only for } t < 0\,,\ n = -1, -2, \ldots\,. \tag{160}$$

If we define the complex delta function at z_n by

$$\int_0^\infty dE\, f(E)\delta(E - z_n) = f(z_n)\,, \tag{161}$$

one can use the results of Lecture 4 to show that the Gamow eigenfunction $u(r;z_n)$, the complex delta function (multiplied by a normalization factor) and the Breit-Wigner amplitude (multiplied by a normalization factor) are linked with each other:

$$\begin{array}{ccccc} u(r;z_n) & \leftrightarrow & i\sqrt{2\pi}\mathscr{N}_n\delta(E - z_n)\,,\ E \in [0, \infty) & \leftrightarrow & -\frac{\mathscr{N}_n}{\sqrt{2\pi}}\frac{1}{E - z_n}\,,\ E \in (-\infty, \infty) \\ \text{posit. repr.} & & \text{energy repr.} & & (-\infty, \infty)\text{-“energy” repr.} \end{array} \tag{162}$$

where

$$\mathscr{N}_n^2 = i\,\mathrm{res}[S(z)]_{z=z_n}\,. \tag{163}$$

Physically, these links mean that the Gamow states yield a decay amplitude $\mathscr{A}(z_{\mathrm{R}} \to E)$ given by the complex delta function, and that such decay amplitude can be approximated by the Breit-Wigner amplitude when we can ignore the lower bound of the energy, i.e., when the resonance is so far from the threshold that we can safely assume that the energy runs over the full real line:

$$\mathscr{A}(z_n \to E) = \langle^- E|z_n\rangle = i\sqrt{2\pi}\mathscr{N}_n\delta(E - z_n) \simeq -\frac{\mathscr{N}_n}{\sqrt{2\pi}}\frac{1}{E - z_n}\,. \tag{164}$$

Thus, the almost-Lorentzian peaks in cross sections are caused by intermediate, unstable particles. However, because there is actually a lower bound for the energy, the decay amplitude is never exactly given by the Breit-Wigner amplitude. This means, in particular, that the standard Gamow states are different from the so-called "Gamow vectors" of [2].

Resonance expansions

The scattering bras and kets are basis vectors that furnish the completeness relation (4). The Gamow states are also basis vectors. The completeness relation (5) generated by the Gamow states is called the resonance expansion.

Resonance expansions are almost always obtained in the same way. One starts from the expansion in terms of bound and scattering states and then, by deforming the continuum integral into the complex plane, and by Cauchy's theorem, one extracts the contributions from the resonances that are hidden in the continuum and write them in the same way as the contributions from the bound states.

For the sake of simplicity, we will focus on the resonance expansion of the transition amplitude from an "in" state φ^+ into an "out" state φ^-:

$$\left(\varphi^-,\varphi^+\right)=\int_0^\infty dE\,\langle\varphi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle\,. \tag{165}$$

We now extract the resonance contributions out of (165) by deforming the contour of integration into the lower half plane of the second sheet of the Riemann surface, where the resonance poles are located, and by applying Cauchy's theorem. Assuming that the integrand $\langle\varphi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle$ tends to zero in the infinite arc of the lower half plane of the second sheet, the resulting resonance expansion is

$$\left(\varphi^-,\varphi^+\right)=\sum_{n=1}^{\infty}\langle\varphi^-|z_n\rangle\langle z_n|\varphi^+\rangle+\int_0^{-\infty} dE\,\langle\varphi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle\,. \tag{166}$$

The integral in Eq. (166) is supposed to be done infinitesimally below the negative real semiaxis of the second sheet. By omitting the wave functions in (166), we obtain the completeness relation (5). In Eq. (166), the infinite sum contains the contribution from the resonances, while the integral is the non-resonant background. Note that in (166) bound states do not appear, since the potential (78) doesn't bind any.

In obtaining Eq. (166), we have assumed that the integrand $\langle\varphi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle$ tends to zero in the infinite arc of the lower half plane of the second sheet. Since (166) makes physical sense, we are tempted to conclude that such must be the case. However, as showed in [9], $\langle\varphi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle$ does not tend to zero in the infinite arc of the lower half plane of the second sheet. On the contrary, it diverges exponentially there. Therefore, Eq. (166) doesn't make sense as it stands. In order to make sense of it, one has to control the exponential blowup of $\langle\varphi^-|E^-\rangle S(E)\langle^+E|\varphi^+\rangle$. The way to do so is by introducing an exponentially damping regulator $e^{-i\alpha z}$, $\alpha>0$. Thus, Eq. (166) should read

$$\left(\varphi^-, \varphi^+\right) = \lim_{\alpha \to 0} \sum_{n=1}^{\infty} e^{-i\alpha z_n} \langle \varphi^- | z_n \rangle \langle z_n | \varphi^+ \rangle + \int_0^{-\infty} dE \, e^{-i\alpha E} \langle \varphi^- | E^- \rangle S(E) \langle {}^+E | \varphi^+ \rangle . \tag{167}$$

Physically, the regulator $e^{-i\alpha z}$ is simply the analytic continuation of the time evolution operator in the energy representation, $e^{-iz\alpha} \equiv e^{-izt/\hbar}$. Thus, the above regularized equation must be understood in a time-asymmetric, time-dependent fashion as

$$(\varphi^-, e^{-iH\frac{t}{\hbar}} \varphi^+) = \sum_{n=1}^{\infty} e^{-iz_n\frac{t}{\hbar}} \langle \varphi^- | z_n \rangle \langle z_n | \varphi^+ \rangle + \int_0^{-\infty} dE \, e^{-iE\frac{t}{\hbar}} \langle \varphi^- | E^- \rangle S(E) \langle {}^+E | \varphi^+ \rangle \tag{168}$$

for $t > 0$ only. Equation (166) should then be seen as the (singular) limit of Eq. (168) when $t \to 0^+$. That for resonances $t \equiv \alpha\hbar$ must be positive is in accord with the time asymmetry of (158).

Expansions (167) and (168) are the reason why we chose a Gaussian falloff for the elements of $\Phi_{\rm exp}$: When the wave functions have a Gaussian falloff in the position representation, we can regularize their blowup in the energy representation and interpret the regulator as a time-asymmetric evolution.

Resonance expansions allow us to understand the deviations from exponential decay. When a particular resonance, say resonance 1, is dominant, then the Gamow state of resonance 1 will carry the exponential decay, whereas the background, which includes in this case also the contribution from other possible resonances, carries the deviations from exponential decay.

The full account of this lecture will appear in a forthcoming paper.

CONCLUSIONS

We have seen why the rigged Hilbert space, rather than the Hilbert space alone, is needed to formulate quantum mechanics when the observables have continuous and/or resonance spectra. The rigged Hilbert space captures the physics of continuous and resonance spectra better than the Hilbert space, because in the rigged Hilbert space physical quantities such as commutation relations, uncertainty principles and resonances have always a precise meaning.

In addition to provide the mathematical support for Dirac's bra-ket formalism, for the Lippmann-Schwinger equation and for the Gamow states, the rigged Hilbert space can be used to obtain the resonance (decay) amplitude in terms of the complex delta function. Such decay amplitude can be approximated by the Breit-Wigner amplitude when the lower bound of the energy can be ignored.

To finish, I would like to mention that there is still a long list of pending questions worth pursuing, such as the invariance properties of $\Phi_{\rm exp}$ under time evolution or a detailed proof of the asymmetry in the time evolution of the Gamow states.

ACKNOWLEDGMENTS

It is a pleasure to thank the organizers for their invitation to participate in this summer school and Oscar Rosas-Ortiz for his hospitality. This work was supported by MEC fellowship No. SD2004-0003.

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