S-matrices

R. Li

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In particle physics, the S-matrix is an object of great interest. In QFT, it is abstractly indexed by asymptotically free incoming and outgoing particles, and is distribution valued. We calculate the entries of these matrices perturbatively using the celebrated Feynman diagrams, or if we're lucky and our system is integrable, we have the chance to calculate these entries exactly.

The distribution can be used to calculate scattering amplitudes, which we use to make predictions about particle interactions. Then, we smash some particles together and check the predictions are correct to ensure we're not wasting our time with these high-energy physics calculations.

1 S-matrix in one dimension: A linear algebra treatment

Consider the time-independent Schrödinger equation (the equation of motion for wavefunctions), for a complex function $\psi : \mathbb{R} \to \mathbb{C}$,

$$-\partial_x^2 \psi + V(x)\psi = E\psi \tag{1}$$

with various factors scaled to make the constants simple. We assume that $V(x)$ decays quickly outside a compact region.

This second order DE in ψ has a solution space generally dependent on E, which we'll label explicitly as $V(E)$, a two-dimensional vector space over $\mathbb{C}$, not to be confused with the potential, $V(x)$, and deliberately not named $H(E)$ as here it is not clear that the solution space is a Hilbert space; indeed for $V(x) \equiv 0$, the solutions are $e^{\pm ikx}$, with k depending on E. The usual norm for functions certainly does not converge.

1.1 Bases for the solution space

We can pick a preliminary basis, $\{\psi_1(x), \psi_2(x)\}$. To make it more explicit that these are vectors in our solution space $V(E)$, we use bra-ket notation $\mathcal{B} = \{|\psi_1\rangle, |\psi_2\rangle\}$. This basis allows us to identify the space of solutions with $\mathbb{C}^2$, via the component map

$$\begin{bmatrix} a \\ b \end{bmatrix} \mapsto a\,|\psi_1\rangle + b\,|\psi_2\rangle \tag{2}$$

which is a linear isomorphism.

Now we quote asymptotics: since $V(x)$ decays at $|x| \to \infty$, we suppose that solutions tend to linear combinations of $e^{\pm ikx}$ at spatial infinity. Hence, assuming generically that there is no degeneracy at $x \to \pm\infty$, we can find linear combinations of the solutions $\{\psi_1(x), \psi_2(x)\}$ satisfying

$$\begin{aligned} \psi_{IN,L}(x) &\to e^{-ikx} \text{ as } x \to -\infty \\ \psi_{OUT,L}(x) &\to e^{-ikx} \text{ as } x \to +\infty \\ \psi_{IN,R}(x) &\to e^{+ikx} \text{ as } x \to +\infty \\ \psi_{OUT,R}(x) &\to e^{+ikx} \text{ as } x \to -\infty \end{aligned} \tag{3}$$

with the physical interpretation of a beam of particles coming in/out from the left/right. We now make the further assumption that the following are good bases, and generically they should be: define

$$\begin{aligned} \mathcal{B}_{IN} &= \{|IN, L\rangle, |IN, R\rangle\} \\ \mathcal{B}_{OUT} &= \{|OUT, L\rangle, |OUT, R\rangle\} \end{aligned} \tag{4}$$

and we have corresponding component maps

$$\begin{aligned} C_{IN} : \begin{bmatrix} A \\ D \end{bmatrix} &\mapsto A\,|IN, L\rangle + D\,|IN, R\rangle \\ C_{OUT} : \begin{bmatrix} B \\ C \end{bmatrix} &\mapsto B\,|OUT, L\rangle + C\,|OUT, R\rangle \end{aligned} \tag{5}$$

1.2 Change of basis

Now given a general solution $|\Psi\rangle$, with our two different bases we can expand in two ways:

$$|\Psi\rangle = A\,|IN, L\rangle + D\,|IN, R\rangle = B\,|OUT, L\rangle + C\,|OUT, R\rangle \tag{6}$$

where B, C is linearly related to A, D via a change of basis matrix. **This is the S-matrix**. Note the usual annoying thing of basis vectors and vector components transforming oppositely: if

$$\begin{aligned} |IN, L\rangle &= S_{11}\,|OUT, L\rangle + S_{21}\,|OUT, R\rangle \\ |IN, R\rangle &= S_{12}\,|OUT, L\rangle + S_{22}\,|OUT, R\rangle \end{aligned} \tag{7}$$

then

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix} = \mathbf{S} \begin{bmatrix} A \\ D \end{bmatrix} \tag{8}$$

note that

$$C_{IN} : \mathbb{C}^2 \to V(E), C_{OUT} : \mathbb{C}^2 \to V(E) \tag{9}$$

are both isomorphisms, so together define a map

$$C_{OUT}^{-1} \circ C_{IN} =: \hat{S} : \mathbb{C}^2 \to \mathbb{C}^2 \tag{10}$$

interpreted as taking components for in states to components for out states, and as a matrix has the components of the S-matrix.

1.3 Unitarity of the S-matrix

Taking the usual norm on $\mathbb{C}^2$, we will show that this $\hat{S}$ map is an isometry, and isometries on complex inner product spaces are unitary, so we conclude that the S-matrix is unitary. We rearrange equation 6:

$$A\,|IN, L\rangle - B\,|OUT, L\rangle = C\,|OUT, R\rangle - D\,|IN, R\rangle =: |\Psi'\rangle \tag{11}$$

From a physical perspective, this is an odd thing to do. This is no longer the same wavefunction as the one we were originally considering.

But this new wavefunction has a big benefit: its asymptotics are very easy to understand. We can read off its asymptotics at $-\infty$ using the left-hand side, and at $+\infty$ using the right-hand side.

Now, the trick that allows us to show the isometry: the probability current,

$$j(x) \propto \psi^* \partial_x \psi - \psi \partial_x \psi^* \tag{12}$$

is constant. We can verify that it is conserved using the equation of motion.

Then, if we evaluate the probability current of $|\Psi'\rangle$ at large $|x|$, for $x << 0$ using the LHS, and $x >> 0$ using the RHS, we get

$$|A|^2 - |B|^2 = |C|^2 - |D|^2 \tag{13}$$

and rearranging gives

$$\text{norm} \begin{bmatrix} A \\ D \end{bmatrix} = \text{norm} \begin{bmatrix} B \\ C \end{bmatrix} \tag{14}$$

hence the $\hat{S}$ map is an isometry of the standard complex inner product, hence is unitary.

1.4 Remarks

In general, this matrix will depend on the parameter E.

The classical system with Hamiltonian $H = \frac{p^2}{2m} + V(x)$ is integrable in the Arnol'd Liouville sense, since we are in 2 dimensions and so only need one conserved quantity, given by $H(x, p)$ itself.