

2.3: Green's Function Analysis of Scattering Resonances

Quasi-bound states and resonances are not limited to 1D, but are equally (or more) important in 2D and 3D. A useful and general way to study them is the quantum Green's function formalism developed in the previous chapter.

Let $\hat{H} = \hat{T} + \hat{V}$ be the Hamiltonian of a system supporting resonances, where \hat{T} is the kinetic energy operator and \hat{V} is the potential operator. We decompose the potential into

$$\hat{V} = \hat{V}_0 + \hat{V}_1, \quad (2.3.1)$$

where \hat{V}_0 is a “confining potential” that supports a bound state, and \hat{V}_1 is a “deconfining potential” that turns the bound state into a quasi-bound state. The figure below shows an example of such a decomposition, for the 1D model from the previous section.

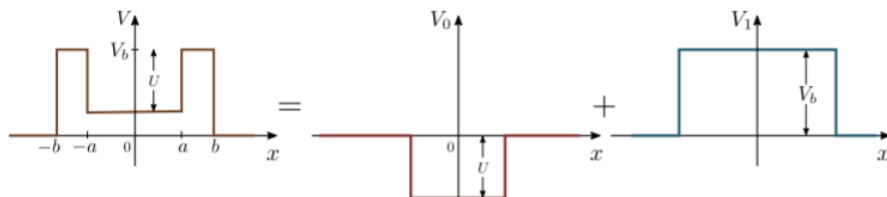


Figure 2.3.1

For the potential \hat{V}_0 (in the absence of \hat{V}_1), let there be a bound state $|\varphi\rangle$, with energy E_0 . Furthermore, we assume that the potential supports a continuum of free states $\{|\psi_k\rangle\}$ with energies $\{E_k\}$, where k is some d -dimensional continuous index for the free states (analogous to the wave-vector for plane wave states). The bound state and free states satisfy the Schrödinger equation

$$(\hat{T} + \hat{V}_0)|\varphi\rangle = E_0|\varphi\rangle \quad (2.3.2)$$

$$(\hat{T} + \hat{V}_0)|\psi_k\rangle = E_k|\psi_k\rangle, \quad (2.3.3)$$

along with the orthogonality and completeness relations

$$\langle\varphi|\psi_k\rangle = 0, \quad |\varphi\rangle\langle\varphi| + \int d^d k |\psi_k\rangle\langle\psi_k| = \hat{I}. \quad (2.3.4)$$

As described in Section 1.7, the causal Green's function is

$$\hat{G}_0(E) = \lim_{\varepsilon \rightarrow 0^+} (E - \hat{T} - \hat{V}_0 + i\varepsilon)^{-1}. \quad (2.3.5)$$

Now introduce the deconfining potential \hat{V}_1 . According to Dyson's equations (Section VI of the previous chapter), the Green's function for the full system is

$$\hat{G} = \hat{G}_0 + \hat{G}\hat{V}_1\hat{G}_0. \quad (2.3.6)$$

We want the matrix elements of $\hat{G}(E)$, which can then be used to find scattering amplitudes. We will calculate them by using the states $|\varphi\rangle$ and $\{|\psi_k\rangle\}$ as a basis—but note that this basis does *not* consist of energy eigenfunctions of the full Hamiltonian \hat{H} . In particular, $|\varphi\rangle$ is not an exact eigenstate of \hat{H} .

As usual when dealing with Dyson's equations, we must watch out for the fact that \hat{G} appears on both the left and right hand sides. This can be dealt with by judiciously inserting a resolution of the identity:

$$\begin{aligned} \hat{G} &= \hat{G}_0 + \hat{G}\hat{I}\hat{V}_1\hat{G}_0 \\ &= \hat{G}_0 + \hat{G} \left(|\varphi\rangle\langle\varphi| + \int d^d k |\psi_k\rangle\langle\psi_k| \right) \hat{V}_1\hat{G}_0. \end{aligned} \quad (2.3.7)$$

We now compute the matrix element $\langle\varphi|\cdots|\varphi\rangle$ for both sides of the equation:

$$\begin{aligned}
 \langle \varphi | \hat{G} | \varphi \rangle &= \langle \varphi | \hat{G}_0 | \varphi \rangle + \langle \varphi | \hat{G} | \varphi \rangle \langle \varphi | \hat{V}_1 \hat{G}_0 | \varphi \rangle + \int d^d k \langle \varphi | \hat{G} | \psi_k \rangle \langle \psi_k | \hat{V}_1 \hat{G}_0 | \varphi \rangle \\
 \langle \varphi | \hat{G} | \varphi \rangle \left(1 - \langle \varphi | \hat{V}_1 \hat{G}_0 | \varphi \rangle \right) &= \langle \varphi | \hat{G}_0 | \varphi \rangle + \int d^d k \langle \varphi | \hat{G} | \psi_k \rangle \langle \psi_k | \hat{V}_1 \hat{G}_0 | \varphi \rangle \\
 \lim_{\varepsilon \rightarrow 0^+} \langle \varphi | \hat{G} | \varphi \rangle \left(1 - \frac{\langle \varphi | \hat{V}_1 | \varphi \rangle}{E - E_0 + i\varepsilon} \right) &= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{E - E_0 + i\varepsilon} \left(1 + \int d^d k \langle \varphi | \hat{G} | \psi_k \rangle \langle \psi_k | \hat{V}_1 | \varphi \rangle \right) \\
 \lim_{\varepsilon \rightarrow 0^+} \langle \varphi | \hat{G} | \varphi \rangle \left(E - E_0 - \langle \varphi | \hat{V}_1 | \varphi \rangle + i\varepsilon \right) - \int d^d k \langle \varphi | \hat{G} | \psi_k \rangle \langle \psi_k | \hat{V}_1 | \varphi \rangle &= 1.
 \end{aligned} \tag{2.3.8}$$

Similarly, computing the matrix element $\langle \varphi | \dots | \psi_k \rangle$ gives:

$$\begin{aligned}
 \langle \varphi | \hat{G} | \psi_k \rangle &= \langle \varphi | \hat{G}_0 | \psi_k \rangle + \langle \varphi | \hat{G} | \varphi \rangle \langle \varphi | \hat{V}_1 \hat{G}_0 | \psi_k \rangle + \int d^d k' \langle \varphi | \hat{G} | \psi_{k'} \rangle \langle \psi_{k'} | \hat{V}_1 \hat{G}_0 | \psi_k \rangle \\
 &= \lim_{\varepsilon \rightarrow 0^+} (E - E_k + i\varepsilon)^{-1} \left(\langle \varphi | \hat{G} | \varphi \rangle \langle \varphi | \hat{V}_1 | \psi_k \rangle + \int d^d k' \langle \varphi | \hat{G} | \psi_{k'} \rangle \langle \psi_{k'} | \hat{V}_1 | \psi_k \rangle \right).
 \end{aligned} \tag{2.3.9}$$

The equations thus far have been exact (we have *not* used perturbation theory). Now we apply an approximation: in the last line of the above equation, let the factor of $\langle \varphi | \hat{G} | \varphi \rangle$ be large, so that the first term in the sum becomes dominant. It will be shown below that $\langle \varphi | \hat{G} | \varphi \rangle$ being large is precisely the resonance condition, so this approximation will be self-consistent. With this, we obtain

$$\langle \varphi | \hat{G} | \psi_k \rangle \approx \lim_{\varepsilon \rightarrow 0^+} \frac{\langle \varphi | \hat{G} | \varphi \rangle \langle \varphi | \hat{V}_1 | \psi_k \rangle}{E - E_k + i\varepsilon}. \tag{2.3.10}$$

Combining this with Equation (2.3.8) gives

$$\lim_{\varepsilon \rightarrow 0^+} \left[\langle \varphi | \hat{G} | \varphi \rangle \left(E - E_0 - \langle \varphi | \hat{V}_1 | \varphi \rangle + i\varepsilon \right) - \int d^d k \frac{\langle \varphi | \hat{G} | \varphi \rangle \langle \varphi | \hat{V}_1 | \psi_k \rangle}{E - E_k + i\varepsilon} \langle \psi_k | \hat{V}_1 | \varphi \rangle \right] \approx 1. \tag{2.3.11}$$

Hence,

Definition: Resonance Condition

$$\begin{aligned}
 \langle \varphi | \hat{G}(E) | \varphi \rangle &\approx \frac{1}{E - E_0 - \langle \varphi | \hat{V}_1 | \varphi \rangle - \Sigma(E)} \\
 \text{where } \Sigma(E) &\equiv \lim_{\varepsilon \rightarrow 0^+} \int d^d k \frac{|\langle \psi_k | \hat{V}_1 | \varphi \rangle|^2}{E - E_k + i\varepsilon}.
 \end{aligned} \tag{2.3.12}$$

The quantity $\Sigma(E)$ is called the **self-energy**, and we will have more to say about it shortly. It depends on E , but let us assume for now that the dependence is weak, so that Σ can be effectively treated as a constant. It is complex-valued, and both its real and imaginary parts are important; we will shortly show that $\text{Im}(\Sigma) < 0$.

From Equation (2.3.12), we can see that $\langle \varphi | \hat{G}(E) | \varphi \rangle$ is large when the denominator is as close to zero as possible. This is called the **resonance condition**, and is self-consistent with the approximation that we made in the above derivation. As we vary the incident energy E over the range of real values, the resonance condition is satisfied when

$$E \approx E_{\text{res}} \equiv E_0 + \langle \varphi | \hat{V}_1 | \varphi \rangle + \text{Re}[\Sigma]. \tag{2.3.13}$$

We call E_{res} the **resonance energy**. Its first term is the energy of the original bound state, in the absence of the deconfining potential \hat{V}_1 . The second term is the energy shift induced by \hat{V}_1 . The third term is equal to the real part of the self-energy Σ , and has a more subtle meaning. Since the definition of Σ involves $\{|\psi_k\rangle\}$, we can think of this term as an energy shift induced by the continuum of free states.

In Section 1.8, we derived the following relationship between the Green's function and the scattering amplitude f :

$$f(\mathbf{k} \rightarrow \mathbf{k}') \propto \langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle + \langle \mathbf{k}' | \hat{V} \hat{G} \hat{V} | \mathbf{k} \rangle. \tag{2.3.14}$$

Here, $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ are incident and scattered plane-wave states satisfying $|\mathbf{k}| = |\mathbf{k}'|$. The first term describes the lowest-order scattering process (the first Born approximation). The second term contains all second- and higher-order scattering processes. By

inserting resolutions of the identity between each \hat{V} and \hat{G} operator in the second term, we find that f contains a contribution of the form

$$\Delta f(\mathbf{k} \rightarrow \mathbf{k}') \propto \langle \mathbf{k}' | \hat{V} | \varphi \rangle \langle \varphi | \hat{G} | \varphi \rangle \langle \varphi | \hat{V} | \mathbf{k} \rangle = \frac{\langle \mathbf{k}' | \hat{V} | \varphi \rangle \langle \varphi | \hat{V} | \mathbf{k} \rangle}{E - E_{\text{res}} - i \text{Im}[\Sigma]} \quad (2.3.15)$$

At resonance, the denominator becomes small and hence Δf should be the dominant contribution to f . It is worth emphasizing that Δf is extracted from a combination of *all* terms in the Born series, not just low-order terms. Intuitively, we can think of a resonant scattering scenario as one where the particle bounces around inside the potential many times before it finally escapes—i.e., high orders in the Born series are significant.

The figure below shows the energy dependence of Δf , according to Equation (2.3.15):

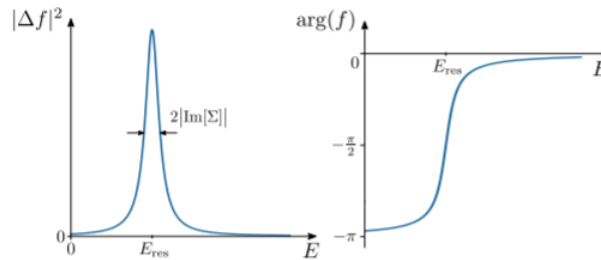


Figure 2.3.2

The graph of $|\Delta f|^2$ versus E has a shape known as a **Lorentzian**. It has a peak centered at the resonance energy E_{res} . The peak width is characterized by the **full-width at half-maximum** (FWHM), the spacing between the two energies where $|\Delta f|^2$ is at half its maximum value:

$$\delta E^{(\text{FWHM})} = 2 |\text{Im}[\Sigma]|. \quad (2.3.16)$$

Thus, the closer the self-energy gets to being a real quantity, the sharper the peak.

The phase $\arg[\Delta f]$ also contains useful information. As E crosses E_{res} from below, the phase increases by π . The energy range over which this phase shift occurs is $\sim |\text{Im}[\Sigma]|$.

These two signatures—peaks and phase shifts—are sought after in numerous real-world scattering experiments. In actual experiments, the peaks and phase shifts are often overlaid on a “background” caused by non-resonant effects. For example, the plot below was released by the CMS experiment at the Large Hadron Collider (LHC), showing a resonance peak on a large background. This was part of the evidence for the LHC’s discovery of a new particle, the Higgs boson, in 2012.

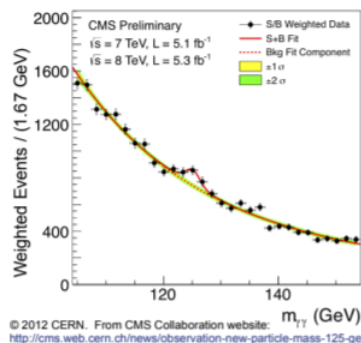


Figure 2.3.3

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