1.11. Fixed-Energy Amplitude

The Fourier-transform of the retarded time evolution amplitude (1.299)

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E^R = \int_{-\infty}^{\infty} d\,t\, e^{i E (t-t')/\hbar} (\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t')^R$$

$$= \int_{t'}^{\infty} d\,t\, e^{i E (t-t')/\hbar} (\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') \qquad (1.313)$$

is called the fixed-energy amplitude.

For a time independent $\hat{H}$,

$$(\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') = \left\langle \boldsymbol{x} \;\middle|\; e^{-i \hat{H} (t-t')/\hbar} \;\middle|\; \boldsymbol{x}' \right\rangle \qquad (1.296)$$

$$\rightarrow \qquad (\boldsymbol{x} \mid \boldsymbol{x}')_E^R = \int_{t'}^{\infty} d\,t \left\langle \boldsymbol{x} \;\middle|\; e^{i\left(E - \hat{H} + i\,\eta\right)(t-t')/\hbar} \;\middle|\; \boldsymbol{x}' \right\rangle$$

$$= \left\langle \boldsymbol{x} \;\middle|\; \frac{i\,\hbar}{E - \hat{H} + i\,\eta} \;\middle|\; \boldsymbol{x}' \right\rangle$$

$$= \left\langle \boldsymbol{x} \;\middle|\; \hat{R}(E + i\,\eta) \;\middle|\; \boldsymbol{x}' \right\rangle \qquad (1.314)$$

where the infinitesimal $\eta > 0$ is added to keep the integral well defined and

$$\hat{R}(E) = \frac{i\,\hbar}{E - \hat{H}} \qquad (1.315)$$

is called the resolvent operator. Note that the "retardedness" is now carried by the slight energy shift $E \to E + i\,\eta$.

For a time-dependent $\hat{H}$, (1.296) is replaced by

$$(\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') = \left\langle \boldsymbol{x} \;\middle|\; \hat{U}(t, t') \;\middle|\; \boldsymbol{x}' \right\rangle \qquad (1.298)$$

and we have

$$\hat{R}(E + i\,\eta) = \int_{t'}^{\infty} d\,t\, e^{i (E + i\,\eta)(t-t')/\hbar}\, \hat{U}(t, t')$$

$$= \int_{-\infty}^{\infty} d\,t\, e^{i E (t-t' + i\,\eta)/\hbar}\, \hat{U}^R(t, t') \qquad (1.316)$$

Assume now the time-independent Schrodinger eq. exists and is completely solved

$$\hat{H} \mid n \rangle = E_n \mid n \rangle \qquad (1.317)$$

Using the completeness

$$\sum_n \mid n \rangle \langle n \mid = \hat{1} \qquad (1.318)$$

we can write (1.296) as

$$(\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') = \sum_n \left\langle \boldsymbol{x} \;\middle|\; e^{-i \hat{H} (t-t')/\hbar} \;\middle|\; n \right\rangle \langle n \mid \boldsymbol{x}' \rangle$$

$$= \sum_n e^{-i E_n (t-t')/\hbar} \langle \boldsymbol{x} \mid n \rangle \langle n \mid \boldsymbol{x}' \rangle$$

$$= \sum_n e^{-i E_n (t-t')/\hbar}\, \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}') \qquad (1.319)$$

where

$$\psi_n(\boldsymbol{x}) = \langle \boldsymbol{x} \mid n \rangle \qquad (1.320)$$

The fixed-energy amplitude (1.313) becomes

$$(\boldsymbol{x} \mid \boldsymbol{x}')_E^R = \sum_n \int_{t'}^{\infty} d\,t\, e^{i (E - E_n + i\,\eta)(t-t')/\hbar}\, \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}')$$

$$= \sum_n \frac{i\hbar}{E - E_n + i\eta} \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}') \qquad (1.321)$$
$$= \sum_n R_n(E + i\eta)\, \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}')$$

where

$$R_n(E) = \frac{i\hbar}{E - E_n} \qquad (1.321a)$$

Note that the propagator is just the inverse Fourier transform of (1.313)

$$(\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar}\, e^{-i(E+i\eta)(t-t')/\hbar}\, (\boldsymbol{x} \mid \boldsymbol{x}')_E \qquad (1.322)$$

where the “retardedness” is indicated by the shift $E \to E + i\eta$, i.e., lifting the integration path slightly above the real E axis. From (1.321), we see that we can achieve the same result by the shift $E_n \to E_n - i\eta$, i.e., shifting the poles of $\hat{R}(E)$ slightly below the real E axis. Hence,

$$\psi_n(t) \propto e^{-i(E_n - i\eta)t/\hbar} \propto e^{-\eta t/\hbar} \to 0 \qquad \text{as} \qquad t \to \infty \qquad (1.323)$$

Finally, to complete the circle of argument, we mention that, with all the poles in the lower complex E-plane, the retardedness, $(\boldsymbol{x}\, t \mid \boldsymbol{x}'\, t') = 0$ for $t < t'$, is ensured.

Using the formula [see any text on the “principal values of improper integrals”]

$$\frac{1}{x \pm i\eta} = \mathcal{P}\frac{1}{x} \mp i\pi\,\delta(x) \qquad (1.325)$$

where $\mathcal{P}$ indicates taking the principal value, we can write the discontinuity of $R_n(E)$ across the real E-axis as

$$\Delta R_n(E) \equiv R_n(E + i\eta) - R_n(E - i\eta)$$
$$= \frac{i\hbar}{E - E_n + i\eta} - \frac{i\hbar}{E - E_n - i\eta}$$
$$= 2\pi\hbar\,\delta(E - E_n) \qquad (1.324)$$

For systems with a continuous spectrum, n becomes a continuous label and the line of eigenvalues E_n becomes a branch cut of $R_n(E)$. For a discrete spectrum, the singularity at E_n is a pole and $\lim_{E \to E_n} R_n(E) \to \infty$. In contrast, $R_n(E)$ on a branch cut has a finite value. The singularity exhibits itself as a finite discontinuity in the values of $R_n(E)$ as E crosses the branch cut.

Similarly, the discontinuity of the fixed energy amplitude $(\boldsymbol{x} \mid \boldsymbol{x}')_E$ is given by

$$\Delta(\boldsymbol{x} \mid \boldsymbol{x}')_E \equiv \left\langle \boldsymbol{x} \,\middle|\, \hat{R}(E + i\eta) - \hat{R}(E - i\eta) \,\middle|\, \boldsymbol{x}' \right\rangle$$
$$= \left\langle \boldsymbol{x} \,\middle|\, \frac{i\hbar}{E - \hat{H} + i\eta} - \frac{i\hbar}{E - \hat{H} - i\eta} \,\middle|\, \boldsymbol{x}' \right\rangle$$
$$= \sum_n [\, R_n(E + i\eta) - R_n(E + i\eta)\,]\, \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}')$$
$$= \sum_n \Delta R_n(E)\, \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}')$$
$$= 2\pi\hbar \sum_n \delta(E - E_n)\, \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}') \qquad (1.326a)$$

Hence,

$$\int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar}\, \Delta(\boldsymbol{x} \mid \boldsymbol{x}')_E = \sum_n \int_{-\infty}^{\infty} dE\, \delta(E - E_n)\, \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}')$$
$$= \sum_n \psi_n(\boldsymbol{x})\, \psi_n^*(\boldsymbol{x}')$$

$$= \sum_n \langle \boldsymbol{x} \mid n \rangle \langle n \mid \boldsymbol{x}' \rangle$$
$$= \langle \boldsymbol{x} \mid \boldsymbol{x}' \rangle = \delta(\boldsymbol{x} - \boldsymbol{x}') \qquad (1.326)$$

Expressing these results in operator form, we set

$$\begin{aligned}
\Delta \hat{R}(E) &\equiv \hat{R}(E + i\,\eta) - \hat{R}(E - i\,\eta) \\
&= \frac{i\,\hbar}{E - \hat{H} + i\,\eta} - \frac{i\,\hbar}{E - \hat{H} - i\,\eta} \\
&= \sum_{n,m} \mid n \rangle \langle n \mid \left(\frac{i\,\hbar}{E - \hat{H} + i\,\eta} - \frac{i\,\hbar}{E - \hat{H} - i\,\eta} \right) \mid m \rangle \langle m \mid \\
&= \sum_n \mid n \rangle \left(\frac{i\,\hbar}{E - E_n + i\,\eta} - \frac{i\,\hbar}{E - E_n - i\,\eta} \right) \langle n \mid \\
&= 2\,\pi\,\hbar \sum_n \mid n \rangle\, \delta(E - E_n) \langle n \mid
\end{aligned}$$

$$\rightarrow \qquad \int_{-\infty}^{\infty} \frac{d\,E}{2\,\pi\,\hbar} \Delta \hat{R}(E) = \sum_n \mid n \rangle \langle n \mid = \hat{1} \qquad (1.327)$$

In case the energy spectrum consists of both discrete and continuous parts, the completeness relation may be written as

$$\sum_n \mid n \rangle \langle n \mid + \int d\,\nu \;\mid \nu \rangle \langle \nu \mid = \hat{1} \qquad (1.328)$$