1.10. Time Evolution Amplitude

The matrix elements of the time evolution operator in the x-representaion are called time evolution amplitudes, or propagators :

$$(\boldsymbol{x}, t \mid \boldsymbol{x}', t') \equiv \left\langle \boldsymbol{x} \,\middle|\, \hat{U}(t, t') \,\middle|\, \boldsymbol{x}' \right\rangle \tag{1.295}$$

They give the probability amplitudes of finding the particle at point $\boldsymbol{x}$ at time t given that it was at point $\boldsymbol{x}'$ at time t'.

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

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

Taking the matrix elements of the eq. of motion for $\hat{U}$, (1.265), we have

$$i\hbar \frac{\partial}{\partial t} \left\langle \boldsymbol{x} \,\middle|\, \hat{U}(t, t') \,\middle|\, \boldsymbol{x}' \right\rangle = \left\langle \boldsymbol{x} \,\middle|\, \hat{H}\,\hat{U}(t, t') \,\middle|\, \boldsymbol{x}' \right\rangle$$

$$= \int d^3x'' \left\langle \boldsymbol{x} \mid \hat{H} \mid \boldsymbol{x}'' \right\rangle \left\langle \boldsymbol{x}'' \,\middle|\, \hat{U}(t, t') \,\middle|\, \boldsymbol{x}' \right\rangle$$

$$= \int d^3x''\, H\left(\boldsymbol{x}, \frac{\hbar}{i}\nabla, t\right) \delta(\boldsymbol{x} - \boldsymbol{x}'') \left\langle \boldsymbol{x}'' \,\middle|\, \hat{U}(t, t') \,\middle|\, \boldsymbol{x}' \right\rangle$$

$$\rightarrow \qquad \left[i\hbar \frac{\partial}{\partial t} - H\left(\boldsymbol{x}, \frac{\hbar}{i}\nabla, t\right) \right] (\boldsymbol{x}, t \mid \boldsymbol{x}', t') = 0 \tag{1.297}$$

The retarded time evolution operator is defined as

$$\hat{U}^R(t, t') \equiv \begin{cases} \hat{U}(t, t') & \text{for } t > t' \\ 0 & \text{for } t < t' \end{cases} \tag{1.298}$$

along with the associated retarded time evolution amplitudes

$$(\boldsymbol{x}, t \mid \boldsymbol{x}', t')^R \equiv \left\langle \boldsymbol{x} \,\middle|\, \hat{U}^R(t, t') \,\middle|\, \boldsymbol{x}' \right\rangle \tag{1.299}$$

Using the Heaviside step function,

$$\Theta(t) \equiv \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases} \tag{1.300}$$

we have

$$\hat{U}^R(t, t') = \Theta(t - t')\, \hat{U}(t, t')$$

$$(\boldsymbol{x}, t \mid \boldsymbol{x}', t')^R = \Theta(t - t')\, (\boldsymbol{x}, t \mid \boldsymbol{x}', t') \tag{1.301}$$

It is easily checked that, for any $a > 0$,

$$\int_{-a}^{t} dt'\, \delta(t') = \Theta(t)$$

Hence,

$$\delta(t) = \frac{d\,\Theta(t)}{dt} \tag{1.303}$$

so that

$$\frac{\partial}{\partial t} \hat{U}^R(t, t') = \delta(t - t') + \theta(t - t') \frac{\partial}{\partial t} \hat{U}(t, t') \tag{1.303a}$$

where $\hat{U}(t', t') = 1$ was used.

Taking the matrix elements of (1.303a) and then using (1.297), we get the equation of motion for the retarded propagator,

$$\left[i\hbar\frac{\partial}{\partial t}-H\left(\boldsymbol{x},\ \frac{\hbar}{i}\nabla,\ t\right)\right](\boldsymbol{x},\ t\mid\boldsymbol{x}',\ t')^R = i\hbar\,\delta(t-t')\,\delta(\boldsymbol{x}-\boldsymbol{x}') \qquad (1.304)$$

As can be seen from (1.296), these propagators depend only on the time difference $t - t'$ if $\hat{H}$ is time-independent.

A retarded function

$$f(t) = 0 \qquad \forall\ t < 0 \qquad (1.306a)$$

has a characteristic Fourier transform

$$\tilde{f}(E) \equiv \int_{-\infty}^{\infty} d\,t\, e^{i E t/\hbar} f(t)$$
$$= \int_{0}^{\infty} d\,t\, e^{i E t/\hbar} f(t) \qquad (1.306)$$

Consider now the evaluation of the inverse transform

$$f(t) \equiv \int_{-\infty}^{\infty} \frac{d\,E}{2\pi\hbar}\, e^{-i E t/\hbar}\, \tilde{f}(E)$$

as the real-axis part of a contour integral in the complex E-plane.

For $t < 0$, the contour must be closed in the upper-half plane so that contribution from the great arc vanishes. Hence, (1.306a) is automatically satisfied if $\tilde{f}(E)$ is analytic in the upper-half plane.

Using $\Theta(t)$ as an example, we have

$$\tilde{\Theta}(E) = \frac{i}{E + i\eta} \qquad \eta \to 0^+$$

The single pole in the lower-half plane at $E = -i\eta$ makes

$$\Theta(t) = \int_{-\infty}^{\infty} \frac{d\,E}{2\pi\hbar}\, e^{-i E t/\hbar}\, \frac{i}{E + i\eta} \qquad (1.308)$$
$$= 1 \qquad \text{for } t > 0$$

Note that, the case $t = 0$ is undefined in (1.308), which is why we define Θ using (1.300). On the other hand, we are free to assign any finite value to $\Theta(0)$ without changing the crucial relation (1.303). Kleinert defined 3 different step functions:

$$\begin{matrix}\Theta(t)\\ \Theta^R(t)\\ \overline{\Theta}(t)\end{matrix} \qquad \text{if} \qquad \Theta(0) = \begin{cases} 0 & \text{see (1.300)} \\ 1 & \text{see (1.302)} \\ \frac{1}{2} & \text{see (1.309)} \end{cases}$$

As with the δ-function, Θ is properly a distribution and is used safely only inside an integral, e.g., as the kernel for a linear functional of smooth test functions:

$$\Theta[f] = \int d\,t\,\Theta(t-t')\,f(t') \qquad (1.310)$$

A closely related distribution is

$$\epsilon(t) \equiv \Theta(t) - \Theta(-t) \qquad (1.311)$$
$$= \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t = 0 \\ -1 & \text{for } t < 0 \end{cases} \qquad (1.312)$$

which is independent of the choice of $\Theta(0)$.