

Generalizations: Adding an extra parameter

In the discussion of implementing the Fourier Transform and the Inverse Fourier

Transform, $\Psi(\mathbf{x})$ and $A(\mathbf{q})$, were always described as vectors, indexed by \mathbf{x} and \mathbf{q} respectively. In general, these each could have been described by a matrix, again, with a row index of \mathbf{x} and \mathbf{q} , but with a column index of some independent parameter, like time.

For example, Ψ could have been a matrix. Each column could be for a different time instance:

$$\Psi = \begin{pmatrix} \Psi(x_1, t_1) & \Psi(x_1, t_2) & \dots & \Psi(x_1, t_l) \\ \Psi(x_2, t_1) & \Psi(x_2, t_2) & \dots & \Psi(x_2, t_l) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi(x_n, t_1) & \Psi(x_n, t_2) & \dots & \Psi(x_n, t_l) \end{pmatrix}$$

then, applying the Fourier Transform procedures exactly as described previously, we

would get a matrix $A(\mathbf{q}, t)$ instead of the vector $\vec{A}(\mathbf{q})$:

$$A(\mathbf{q}, t) = \begin{pmatrix} A(q_1, t_1) & A(q_1, t_2) & \dots & A(q_1, t_l) \\ A(q_2, t_1) & A(q_2, t_2) & \dots & A(q_2, t_l) \\ \vdots & \vdots & \ddots & \vdots \\ A(q_m, t_1) & A(q_m, t_2) & \dots & A(q_m, t_l) \end{pmatrix} \Psi(\mathbf{x}, t = 0)$$

The most probable scenario is that we are given the initial wavepacket and wish to find the wave packet at time $t > 0$. In this case we perform the Fourier Transform on a single column, and are returned a single column amplitude function. Then, we want to find Ψ for many time instances. Using matrices instead of vectors, we can compute all the time instances at once. First, we setup a matrix \mathbf{A} :

$$\begin{aligned} \mathbf{A} &= \begin{pmatrix} A(q_1) \\ A(q_2) \\ \vdots \\ A(q_m) \end{pmatrix} * \begin{pmatrix} 1 & 1 & \dots & 1_m \end{pmatrix} \\ &= \begin{pmatrix} A(q_1) & A(q_1) & \dots & A(q_1) \\ A(q_2) & A(q_2) & \dots & A(q_2) \\ \vdots & \vdots & \ddots & \vdots \\ A(q_m) & A(q_m) & \dots & A(q_m) \end{pmatrix} \end{aligned}$$

This is a matrix, with identical column. Each column is the expansion coefficients we computed from the Fourier transform of Ψ . We will put one column in the matrix for each future time instance we wish to compute Ψ at.

$\vec{\zeta}$

If we then similarly redefine $\vec{\zeta}$ to account for the time parameter as follows:

$$\vec{\zeta} = \begin{pmatrix} e^{-iE_1 t_1/\hbar} & e^{-iE_1 t_2/\hbar} & \dots & e^{-iE_1 t_l/\hbar} \\ e^{-iE_2 t_1/\hbar} & e^{-iE_2 t_2/\hbar} & \dots & e^{-iE_2 t_l/\hbar} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-iE_m t_1/\hbar} & e^{-iE_m t_2/\hbar} & \dots & e^{-iE_m t_l/\hbar} \end{pmatrix}$$

Now, if we perform array multiplication (element by element) on $\vec{\zeta}$ and \mathbf{A} we get:

$$\mathbf{A}(q, t) = \begin{pmatrix} A(q_1)e^{-it_1 E_1/\hbar} & A(q_1)e^{-it_2 E_1/\hbar} & A(q_1)e^{-it_3 E_1/\hbar} & \dots & A(q_1)e^{-it_l E_1/\hbar} \\ A(q_2)e^{-it_1 E_2/\hbar} & A(q_2)e^{-it_2 E_2/\hbar} & A(q_2)e^{-it_3 E_2/\hbar} & \dots & A(q_2)e^{-it_l E_2/\hbar} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A(q_m)e^{-it_1 E_m/\hbar} & A(q_m)e^{-it_2 E_m/\hbar} & A(q_m)e^{-it_3 E_m/\hbar} & \dots & A(q_m)e^{-it_l E_m/\hbar} \end{pmatrix}$$

$\vec{\phi}_q * \mathbf{A}(q, t)$

and, if we multiply $\vec{\phi}_q * \mathbf{A}(q, t)$, just like we did in the previous sections:

$$= \begin{pmatrix} (A(q_1, t_1)e^{iq_1 x_1} + \dots + A(q_m, t_1)e^{iq_m x_1}) & \dots & (A(q_1, t_l)e^{iq_1 x_1} + \dots + A(q_m, t_l)e^{iq_m x_1}) \\ (A(q_1, t_1)e^{iq_1 x_2} + \dots + A(q_m, t_1)e^{iq_m x_2}) & \dots & (A(q_1, t_l)e^{iq_1 x_2} + \dots + A(q_m, t_l)e^{iq_m x_2}) \\ \vdots & \vdots & \vdots \\ (A(q_1, t_1)e^{iq_1 x_n} + \dots + A(q_m, t_1)e^{iq_m x_n}) & \dots & (A(q_1, t_l)e^{iq_1 x_n} + \dots + A(q_m, t_l)e^{iq_m x_n}) \end{pmatrix}$$

which is just

$$\Psi(x, t) = \begin{pmatrix} \Psi(x_1, t_1) & \Psi(x_1, t_2) & \dots & \Psi(x_1, t_l) \\ \Psi(x_2, t_1) & \Psi(x_2, t_2) & \dots & \Psi(x_2, t_l) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi(x_n, t_1) & \Psi(x_n, t_2) & \dots & \Psi(x_n, t_l) \end{pmatrix}$$