

# s03E01 Scattering theory

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## 1 A useful calculation

$$\begin{aligned} -i \int_{-\infty}^t dt' \langle \psi_j | H_{1I} | \psi_i \rangle &= -i \int_{-\infty}^t dt' e^{-i\omega_{ij}t'} \langle \psi_j | H_1 | \psi_i \rangle \\ &= -i \int_{-\infty}^t dt' e^{-i\omega_{ij}t'} \langle \psi_j | H_1 | \psi_i \rangle e^{0^+ t} \\ &= \frac{1}{\omega_{ij} + i0^+} e^{-i\omega_{ij}t'} \langle \psi_j | H_1 | \psi_i \rangle e^{0^+ t} \\ &= \frac{1}{\omega_{ij} + i0^+} e^{-i\omega_{ij}t'} \langle \psi_j | H_1 | \psi_i \rangle \end{aligned}$$

## 2 The scattering $S$ - and $T$ -matrix

The scattering  $S$ -matrix is defined by

$$S \equiv U_{+\infty -\infty}$$

We have, using the useful calculation above,

$$S_{ji} = \langle \psi_j | U_{+\infty -\infty} | \psi_i \rangle = \delta_{ji} - iT_{ji} 2\pi \delta^1(\omega_{ij})$$

where the  $T$ -matrix is given by the so-called **old-fashioned perturbation theory**

$$T = V + V \frac{1}{E_i - H_0 + i0^+} V + V \frac{1}{E_i - H_0 + i0^+} V \frac{1}{E_i - H_0 + i0^+} V + \dots$$

and is related to the transition probability

$$p_{i \rightarrow j} = |T_{ji}|^2 2\pi t \delta^1(\omega_{ij})$$

### 3 The Lippmann-Schwinger equation

We define

$$\begin{aligned} |\psi_{i+}\rangle &\equiv U_{0-\infty}|\psi_i\rangle \\ |\psi_{i-}\rangle &\equiv U_{0+\infty}|\psi_i\rangle \end{aligned}$$

or equivalently,

$$\begin{aligned} \lim_{t \rightarrow -\infty} e^{-iHt} |\psi_{i+}\rangle &= \lim_{t \rightarrow -\infty} e^{-iH_0 t} |\psi_i\rangle \\ \lim_{t \rightarrow +\infty} e^{-iHt} |\psi_{i-}\rangle &= \lim_{t \rightarrow +\infty} e^{-iH_0 t} |\psi_i\rangle \end{aligned}$$

and by definition,

$$\begin{aligned} S_{ji} &= \langle \psi_j | U_{+\infty -\infty} | \psi_i \rangle \\ &= \langle \psi_j | U_{+\infty 0} U_{0 -\infty} | \psi_i \rangle \\ &= \langle \psi_{j-} | \psi_{i+} \rangle \end{aligned}$$

To obtain the expression of  $|\psi_{i+}\rangle$ , we use the useful calculation

$$\langle \psi_j | \psi_{i+} \rangle = \langle \psi_j | U_{0-\infty} | \psi_i \rangle = \langle \psi_j | \psi_i \rangle + \langle \psi_j | \frac{1}{E_i - H_0 + i0^+} T | \psi_i \rangle$$

from which we read the Lippmann-Schwinger equation:

$$\begin{aligned} |\psi_{i+}\rangle &= |\psi_i\rangle + \frac{1}{E_i - H_0 + i0^+} T | \psi_i \rangle \\ &= |\psi_i\rangle + \frac{1}{E_i - H_0 + i0^+} V | \psi_{i+} \rangle \end{aligned}$$

Since by definition  $H_0 |\psi_i\rangle = E_i |\psi_i\rangle$ , we have

$$H_0 |\psi_{i+}\rangle + V |\psi_{i+}\rangle = E_i |\psi_{i+}\rangle$$

namely  $|\psi_{i+}\rangle$  is an eigenstate of the total  $H$ , with the same eigenvalue  $E_i$ . Therefore, if  $|\psi_i\rangle$  is a scattering eigenstate of  $H_0$ , then  $|\psi_{i+}\rangle$  is a scattering eigenstate of  $H$ .

### 4 Scattering problem in three dimensions

The scattering problem in three dimensions is a good place to show the usefulness of the Lippmann-Schwinger equation. To set up the problem, notice that the scattering

eigenstates of the free Hamiltonian  $H_0$  are the plane waves, and thus we may take the state  $|\psi_i\rangle$  to be the plane wave with wave vector  $\mathbf{k}_i$ .

We then use the Lippmann-Schwinger equation to calculate the scattering eigenstates of the total Hamiltonian

$$|\psi_{i+}\rangle = |\psi_i\rangle + \frac{1}{E_i - H_0 + i0^+} T |\psi_i\rangle$$

Now let us compute the coordinate space wave function of the scattering eigenstates, and focus on its asymptotic behavior. Noticing the following calculation,

$$\langle \mathbf{x} | \frac{1}{E_i - H_0 + i0^+} | \mathbf{y} \rangle = 2m \int \frac{d^3 \mathbf{l}}{(2\pi)^3} \frac{e^{i\mathbf{l}\cdot\mathbf{x}} e^{-i\mathbf{l}\cdot\mathbf{y}}}{k^2 - l^2 + i0^+} = -\frac{m}{2\pi} \frac{e^{ik_i\eta}}{\eta}$$

where  $\eta$  is the distance between  $\mathbf{x}$  and  $\mathbf{y}$ . In the limit  $x \rightarrow \infty$ , we have

$$\frac{e^{ik_i\eta}}{\eta} = \frac{e^{ik_i r}}{r} e^{-ik_i \mathbf{y} \cdot \hat{\mathbf{x}}} = \frac{e^{ik_i r}}{r} \langle \psi_j | \mathbf{y} \rangle$$

where  $|\psi_j\rangle$  is the plane wave with wave vector  $\mathbf{k}_j = k_i \hat{\mathbf{x}}$ . Thus we read

$$\langle \mathbf{x} | \psi_{i+} \rangle = \langle \mathbf{x} | \psi_i \rangle - \frac{m}{2\pi} \frac{e^{ik_i r}}{r} \langle \psi_j | T | \psi_i \rangle$$

which means that asymptotically, the coordinate space wave function of the scattering eigenstates of the total  $H$  is the superposition of the incoming plane wave  $|\psi_i\rangle$  and an outgoing spherical wave, modulated by an angular distribution function  $-\frac{m}{2\pi} T_{ji}$ . Since we already know that the transition probability is proportional to  $|T_{ji}|^2$ , we now know that it is, equivalently, proportional to the square of the angular distribution function.

## 5 The Wigner-Eckart theorem

The statement of the Wigner-Eckart theorem is quite intuitive: if some operators  $T_{jm}$  transform like the  $|jm\rangle$  states, where  $j$  is fixed, then we have

$$\langle \alpha, jm | T_{j_1 m_1} | \alpha_2, j_2 m_2 \rangle = \langle jm | j_1 m_1, j_2 m_2 \rangle \langle \alpha, j || T_{j_1} || \alpha_2, j_2 \rangle$$

where  $\langle \alpha, j || T_{j_1} || \alpha_2, j_2 \rangle$  is a number that does not depend on  $m, m_1$  or  $m_2$ .

## 6 Rotational symmetry

In the special case that the scattering potential  $V$  is rotationally invariant, the general non-perturbative analysis above can be carried out further. In this case, the total  $H$  is rotationally invariant, and thus the scattering  $S$ - and  $T$ -matrices are rotationally invariant. In other words, they are scalar operators. The Wigner-Eckart theorem:

$$\begin{aligned}\langle E, lm | S | E', l' m' \rangle &= \delta_{ll'} \delta_{mm'} \langle E, l | S | E', l' \rangle \\ &= \delta_{ll'} \delta_{mm'} \langle E, l | S | E', l \rangle\end{aligned}$$

Since we also know that the result should be proportional to  $\delta_{EE'}$ , we arrive at the conclusion that the scattering  $S$ -matrix is diagonal in the  $|E, lm\rangle$  basis, with diagonal elements depending only on  $E$  and  $l$ ,

$$\langle E, lm | S | E', l' m' \rangle = \delta_{ll'} \delta_{mm'} \delta_{EE'} S_{E,l}$$

and due to unitarity, the diagonal element  $S_{E,l}$  can only be a phase.

The  $T$ -matrix is also a scalar operator, and we have, considering the case  $E' = E$ ,

$$\begin{aligned}\langle E, lm | T | E, l' m' \rangle &= \delta_{ll'} \delta_{mm'} \langle E, l | T | E, l' \rangle \\ &= \delta_{ll'} \delta_{mm'} \langle E, l | T | E, l \rangle \\ &= \delta_{ll'} \delta_{mm'} T_{E,l}\end{aligned}$$

Thus we conclude that

$$S_{E,l} = 1 - 2\pi i T_{E,l}$$

## 7 Spherical harmonics

$$\mathcal{D}_{\phi\theta\psi} |jm\rangle = \mathcal{D}_{\phi\theta\psi, jm'jm} |jm'\rangle$$

We have

$$\begin{aligned}Y_{lm, \hat{\mathbf{n}}*} &= \langle lm | \hat{\mathbf{n}} \rangle \\ &= \langle lm | \mathcal{D}_{\phi\theta\psi} | \hat{\mathbf{z}} \rangle \\ &= \langle lm | \mathcal{D}_{\phi\theta\psi} | l' m' \rangle \langle l' m' | \hat{\mathbf{z}} \rangle \\ &= \langle lm | \mathcal{D}_{\phi\theta\psi} | lm' \rangle \langle lm' | \hat{\mathbf{z}} \rangle \\ &= \langle lm | \mathcal{D}_{\phi\theta\psi} | l0 \rangle \langle l0 | \hat{\mathbf{z}} \rangle \\ &= \mathcal{D}_{\phi\theta\psi, lm l0} Y_{l0, \hat{\mathbf{z}}*}\end{aligned}$$

where  $Y_{l0,\hat{z}} = \sqrt{\frac{2l+1}{4\pi}}$ . This calculation shows that the spherical harmonics are related to the matrix representation of the rotation operators in a simple way. Notice that

$$\mathcal{D}_{\phi\theta\psi,lm l0} = \mathcal{D}_{\phi\theta0,lm l0}$$

We also have

$$\begin{aligned}\langle E, lm | \mathbf{p} \rangle &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | p \hat{\mathbf{z}} \rangle \\ &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | E', l' m' \rangle \langle E', l' m' | p \hat{\mathbf{z}} \rangle \\ &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | E, l m' \rangle \langle E, l m' | p \hat{\mathbf{z}} \rangle \\ &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | E, l 0 \rangle \langle E, l 0 | p \hat{\mathbf{z}} \rangle \\ &= \mathcal{D}_{\phi\theta\psi,lm l0} \langle E, l 0 | p \hat{\mathbf{z}} \rangle\end{aligned}$$