S03E01 Scattering theory

Liqin Huang

1 A useful calculation

$$-i\int_{-\infty}^{t} dt' \langle\psi_j|H_{1I}|\psi_i\rangle = -i\int_{-\infty}^{t} dt' \langle\psi_j|H_1|\psi_i\rangle\, e^{-i\omega_{ij}t'}$$
$$= -i\int_{-\infty}^{t} dt' \langle\psi_j|H_1|\psi_i\rangle\, e^{-i\omega_{ij}t'} e^{0^+ t}$$

2 The scattering S- and T-matrix

The scattering S-matrix is defined by

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

and using the useful calculation above,

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

with the T-matrix given by the so-called **old-fashioned perturbation theory**

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

which is related to the transition rate

$$w_{i\to j} = |T_{ji}|^2\,2\pi\delta^1(\omega_{ij})$$

3 The optical theorem

The S-matrix is unitary, which means that

$$\begin{aligned}\delta_{\gamma\alpha} &= \int d\beta\, S_{\beta\gamma *} S_{\beta\alpha} = \int d\beta\, \left[\delta_{\beta\gamma} + i T_{\beta\gamma *}\, 2\pi\delta^1(\omega_{\gamma\beta})\right]\left[\delta_{\beta\alpha} - i T_{\beta\alpha}\, 2\pi\delta^1(\omega_{\alpha\beta})\right] \\ &= \int d\beta\, S_{\gamma\beta} S_{\alpha\beta *} = \int d\beta\, \left[\delta_{\gamma\beta} - i T_{\gamma\beta}\, 2\pi\delta^1(\omega_{\beta\gamma})\right]\left[\delta_{\alpha\beta} + i T_{\alpha\beta *}\, 2\pi\delta^1(\omega_{\beta\alpha})\right]\end{aligned}$$

from which we obtain, after cancelling a delta function,

$$\begin{aligned} i T_{\gamma\alpha} - i T_{\alpha\gamma *} &= \int d\beta\, T_{\beta\gamma *} T_{\beta\alpha}\, 2\pi\delta^1(\omega_{\alpha\beta}) \\ &= \int d\beta\, T_{\gamma\beta} T_{\alpha\beta *}\, 2\pi\delta^1(\omega_{\beta\gamma})\end{aligned}$$

For the special case $\gamma = \alpha$, we have the **optical theorem**

$$i T_{\alpha\alpha} - i T_{\alpha\alpha *} = \int d\beta\, w_{\alpha\to\beta} = \int d\beta\, w_{\beta\to\alpha}$$

4 The Lippmann-Schwinger equation

We define the in and out states

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

or equivalently,

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

and by definition, the S-matrix element

$$S_{ji} = \langle\psi_j|U_{+\infty-\infty}|\psi_i\rangle = \langle\psi_{j-}|\psi_{i+}\rangle$$

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.

5 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 η is the distance between $\mathbf{x}$ and $\mathbf{y}$. In the limit $x \to \infty$, 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.

$$\operatorname{im} f_{\alpha\to\alpha} = -\frac{m}{2\pi}\operatorname{im} T_{\alpha\alpha} = \frac{m}{4\pi}\int d\beta\, w_{\alpha\to\beta} = \frac{m}{4\pi}\int d\sigma\, J_\alpha = \frac{k_\alpha}{4\pi}\sigma$$

6 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.

7 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

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

8 Spherical harmonics

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

We have

$$\begin{aligned}
Y_{lm,\hat{\mathbf{n}}*} &= \langle lm|\hat{\mathbf{n}}\rangle \\
&= \langle lm|\mathcal{D}_{\phi\theta\psi}|\hat{\mathbf{z}}\rangle \\
&= \langle lm|\mathcal{D}_{\phi\theta\psi}|l'm'\rangle\langle l'm'|\hat{\mathbf{z}}\rangle \\
&= \langle lm|\mathcal{D}_{\phi\theta\psi}|lm'\rangle\langle lm'|\hat{\mathbf{z}}\rangle \\
&= \langle lm|\mathcal{D}_{\phi\theta\psi}|l0\rangle\langle l0|\hat{\mathbf{z}}\rangle \\
&= \mathcal{D}_{\phi\theta\psi,lml0}Y_{l0,\hat{\mathbf{z}}*}
\end{aligned}$$

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

$$\mathcal{D}_{\phi\theta\psi,lml0} = \mathcal{D}_{\phi\theta0,lml0}$$

We also have

$$\begin{aligned}
\langle E,lm|\mathbf{p}\rangle &= \langle E,lm|\mathcal{D}_{\phi\theta\psi}|p\hat{\mathbf{z}}\rangle \\
&= \langle E,lm|\mathcal{D}_{\phi\theta\psi}|E',l'm'\rangle\langle E',l'm'|p\hat{\mathbf{z}}\rangle \\
&= \langle E,lm|\mathcal{D}_{\phi\theta\psi}|E,lm'\rangle\langle E,lm'|p\hat{\mathbf{z}}\rangle \\
&= \langle E,lm|\mathcal{D}_{\phi\theta\psi}|E,l0\rangle\langle E,l0|p\hat{\mathbf{z}}\rangle \\
&= \mathcal{D}_{\phi\theta\psi,lml0}\langle E,l0|p\hat{\mathbf{z}}\rangle
\end{aligned}$$