

Quantum Mechanics II

Scattering (3): Formalities

The Lippmann-Schwinger Equation;
The S-Matrix & the T-Matrix

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Formal Scattering

The Lippmann-Schwinger Equation

- Start with

$$\hat{H} = \hat{H}_0 + \hat{W}$$

“Resolvents”

- then define

$$\hat{G}(z) := [z - \hat{H}]^{-1} \quad \hat{G}_0(z) := [z - \hat{H}_0]^{-1} \quad z \in \mathbb{C}$$

- and

$$\hat{T}(z) : \quad \hat{G}(z) =: \hat{G}_0(z) + \hat{G}_0(z) \hat{T}(z) \hat{G}_0(z)$$

$$\hat{G}_0(z) \hat{T}(z) \hat{G}_0(z) = \hat{G}(z) - \hat{G}_0(z)$$

- From this,

$$\hat{T} \hat{G}_0 = \hat{G}_0^{-1} \hat{G} - \mathbf{1}$$

Formal Scattering

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From this,

$$\hat{T}\hat{G}_0 = \hat{G}_0^{-1}\hat{G} - 1 = \hat{G}_0^{-1}\hat{G} - \hat{G}^{-1}\hat{G} = (\hat{G}_0^{-1} - \hat{G}^{-1})\hat{G}$$

$$= (z - \hat{H}_0 - (z - \hat{H}))\hat{G} = \hat{W}\hat{G} \quad \boxed{\hat{T}\hat{G}_0 = \hat{W}\hat{G}}$$

$$\hat{W}\hat{G} = \hat{G}_0^{-1}\hat{G} - 1 \quad \hat{G}_0\hat{W} = 1 - \hat{G}_0\hat{G}^{-1} \quad \hat{G}_0\hat{G}^{-1} = 1 - \hat{G}_0\hat{W}$$

$$\hat{G}_0\hat{T} = \hat{G}\hat{G}_0^{-1} - 1 = \dots = \hat{G}\hat{W}$$

Formal Scattering

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$$\hat{G}_0\hat{T} = \hat{G}\hat{G}_0^{-1} - 1 = \dots = \hat{G}\hat{W} \quad \hat{G}\hat{G}_0^{-1} = 1 + \hat{G}\hat{W}$$

$$1 = \hat{G}_0\hat{G}^{-1}\hat{G}\hat{G}_0^{-1} = [1 - \hat{G}_0\hat{W}][1 + \hat{G}\hat{W}]$$

Formal Scattering

The Lippmann-Schwinger Equation

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“Resolvents”

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From this,

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$$= (z - \hat{H}_0 - (z - \hat{H}))\hat{G} = \hat{W}\hat{G} \quad \boxed{\hat{T}\hat{G}_0 = \hat{W}\hat{G}}$$

$$\hat{W}\hat{G} = \hat{G}_0^{-1}\hat{G} - \mathbf{1} \quad \hat{G}_0\hat{W} = \mathbf{1} - \hat{G}_0\hat{G}^{-1} \quad \hat{G}_0\hat{G}^{-1} = \mathbf{1} - \hat{G}_0\hat{W}$$

$$\hat{G}_0\hat{T} = \hat{G}\hat{G}_0^{-1} - \mathbf{1} = \dots = \hat{G}\hat{W} \quad \hat{G}\hat{G}_0^{-1} = \mathbf{1} + \hat{G}\hat{W}$$

$$1 = \hat{G}_0\hat{G}^{-1}\hat{G}\hat{G}_0^{-1} = [\mathbf{1} - \hat{G}_0\hat{W}][\mathbf{1} + \hat{G}\hat{W}] \quad \boxed{[\mathbf{1} + \hat{G}\hat{W}] = [\mathbf{1} - \hat{G}_0\hat{W}]^{-1}}$$

Formal Scattering

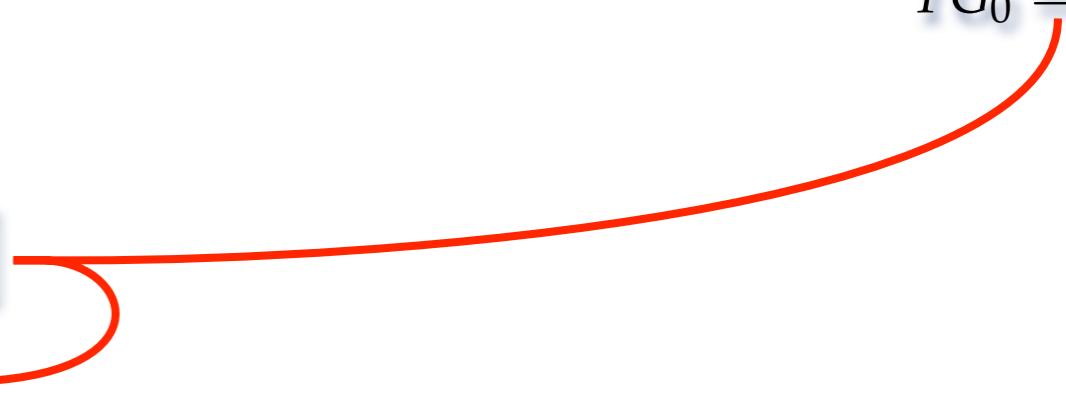
The Lippmann-Schwinger Equation

$$[\mathbb{1} + \hat{G}\hat{W}] = [\mathbb{1} - \hat{G}_0\hat{W}]^{-1}$$

$$\hat{T}\hat{G}_0 = \hat{W}\hat{G}$$

- Now use this:

$$\begin{aligned}\hat{G}(z) &= [\hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)] \\ &= \hat{G}_0(z) + \hat{G}_0(z)\hat{W}(z)\hat{G}(z)\end{aligned}$$



Formal Scattering

The Lippmann-Schwinger Equation

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$$\begin{aligned}
 \hat{G}(z) &= [\hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)] \\
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Formal Scattering

The Lippmann-Schwinger Equation

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$$\hat{G}(z) = [\hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)]$$

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$$= \hat{G}_0(z) + \hat{G}_0(z)\hat{W}(z)[\hat{G}_0(z) + \hat{G}_0(z)\hat{W}(z)\hat{G}(z)]$$

$$= \hat{G}_0(z) + \hat{G}_0(z)\hat{W}(z)\hat{G}_0(z) + \hat{G}_0(z)\hat{W}(z)\hat{G}_0(z)\hat{W}(z)\hat{G}(z)$$

$$\hat{G}(z) = \hat{G}_0 + \hat{G}_0\hat{W}\hat{G}_0 + \hat{G}_0\hat{W}\hat{G}_0\hat{W}\hat{G}_0 + \hat{G}_0\hat{W}\hat{G}_0\hat{W}\hat{G}_0\hat{W}\hat{G}_0 + \dots$$

- This computes the resolvent of the full Hamiltonian iteratively.
- The T-operator is then expressed similarly:

$$\hat{T}(z) = \hat{W}\hat{G}\hat{G}_0^{-1}$$

Formal Scattering

$$[\mathbb{1} + \hat{G}\hat{W}] = [\mathbb{1} - \hat{G}_0\hat{W}]^{-1}$$

The Lippmann-Schwinger Equation

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- Now use this:

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 \hat{G}(z) &= [\hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)] \\
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Formal Scattering

$$[\mathbf{1} + \hat{G}\hat{W}] = [\mathbf{1} - \hat{G}_0\hat{W}]^{-1}$$

The Lippmann-Schwinger Equation

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- Now use this:

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 \hat{G}(z) &= [\hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)] \\
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 \hat{T}(z) &= \hat{W}\hat{G}\hat{G}_0^{-1} = \hat{W}[\hat{G}_0 + \hat{G}_0\hat{W}\hat{G}_0 + \hat{G}_0\hat{W}\hat{G}_0\hat{W}\hat{G}_0 + \dots]\hat{G}_0^{-1} \\
 &= \hat{W}[\mathbf{1} + \hat{G}_0\hat{W} + \hat{G}_0\hat{W}\hat{G}_0\hat{W} + \hat{G}_0\hat{W}\hat{G}_0\hat{W}\hat{G}_0\hat{W} + \dots] \\
 &= \hat{W} + \hat{W}[\hat{G}_0 + \hat{G}_0\hat{W}\hat{G}_0 + \hat{G}_0\hat{W}\hat{G}_0\hat{W}\hat{G}_0 + \dots]\hat{W} \\
 \hat{T}(z) &= \hat{W} + \hat{W}\hat{G}\hat{W}
 \end{aligned}$$

Formal Scattering

The Lippmann-Schwinger Equation

$$\begin{aligned}\hat{G}_0(z) &:= [z - \hat{H}_0]^{-1} \\ [\mathbb{1} + \hat{G}\hat{W}] &= [\mathbb{1} - \hat{G}_0\hat{W}]^{-1} \\ \hat{T}(z) &= \hat{W} + \hat{W}\hat{G}\hat{W}\end{aligned}$$

So... What does this have to do with scattering?

Well, consider $\hat{H} |\Psi_{\mathbf{a}}^{(+)}\rangle = [\hat{H}_0 + \hat{W}] |\Psi_{\mathbf{a}}^{(+)}\rangle = E |\Psi_{\mathbf{a}}^{(+)}\rangle$

rearrange: $[E - \hat{H}_0] |\Psi_{\mathbf{a}}^{(+)}\rangle = \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle \quad [E - \hat{H}_0]^{-1} = G_0(E^+)$

solve: $|\Psi_{\mathbf{a}}^{(+)}\rangle = |\Phi_{\mathbf{a}}\rangle + \hat{G}_0(E^+) \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle$

Formal Scattering

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rearrange: $[E - \hat{H}_0] |\Psi_a^{(+)}\rangle = \hat{W} |\Psi_a^{(+)}\rangle$ *(a plane wave)*
the homogeneous solution

solve:

$$|\Psi_a^{(+)}\rangle = \underbrace{|\Phi_a\rangle}_{\text{incident}} + \underbrace{\hat{G}_0(E^+) \hat{W} |\Psi_a^{(+)}\rangle}_{\text{scattering out-going}}$$

$$[E - \hat{H}_0] |\Phi_a\rangle = 0$$

$$E^+ := \lim_{\epsilon \rightarrow 0} (E + i\epsilon)_{\epsilon \geq 0}$$

...rearrange

$$|\Phi_a\rangle = |\Psi_a^{(+)}\rangle - \hat{G}_0(E^+) \hat{W} |\Psi_a^{(+)}\rangle = [\mathbb{1} - \hat{G}_0(E^+) \hat{W}] |\Psi_a^{(+)}\rangle$$

...and solve

$$|\Psi_a^{(+)}\rangle = [\mathbb{1} - \hat{G}_0(E^+) \hat{W}]^{-1} |\Phi_a\rangle = [\mathbb{1} + \hat{G}(E^+) \hat{W}] |\Phi_a\rangle$$

Formal Scattering

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$$|\Psi_a^{(+)}\rangle = [\mathbb{1} - \hat{G}_0(E^+) \hat{W}]^{-1} |\Phi_a\rangle = [\mathbb{1} + \hat{G}(E^+) \hat{W}] |\Phi_a\rangle$$

Now,

$$\hat{W} |\Psi_a^{(+)}\rangle = [\hat{W} + \hat{W} \hat{G}(E^+) \hat{W}] |\Phi_a\rangle = \hat{T}(E^+) |\Phi_a\rangle$$

$$\hat{G}_0(z) := [z - \hat{H}_0]^{-1}$$

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Formal Scattering

The Lippmann-Schwinger Equation

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rearrange: $[E - \hat{H}_0] |\Psi_{\mathbf{a}}^{(+)}\rangle = \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle$ (a plane wave)
~~the homogeneous solution~~

solve: $|\Psi_{\mathbf{a}}^{(+)}\rangle = \underbrace{|\Phi_{\mathbf{a}}\rangle}_{\text{incident}} + \underbrace{\hat{G}_0(E^+) \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle}_{\text{scattering out-going}}$ $[E - \hat{H}_0] |\Phi_{\mathbf{a}}\rangle = 0$

$E^+ := \lim_{\epsilon \rightarrow 0} (E + i\epsilon)_{\epsilon \geq 0}$

...rearrange

$$|\Phi_{\mathbf{a}}\rangle = |\Psi_{\mathbf{a}}^{(+)}\rangle - \hat{G}_0(E^+) \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle = [\mathbb{1} - \hat{G}_0(E^+) \hat{W}] |\Psi_{\mathbf{a}}^{(+)}\rangle$$

...and solve

$$|\Psi_{\mathbf{a}}^{(+)}\rangle = [\mathbb{1} - \hat{G}_0(E^+) \hat{W}]^{-1} |\Phi_{\mathbf{a}}\rangle = [\mathbb{1} + \hat{G}(E^+) \hat{W}] |\Phi_{\mathbf{a}}\rangle$$

Now,

$$\hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle = [\hat{W} + \hat{W} \hat{G}(E^+) \hat{W}] |\Phi_{\mathbf{a}}\rangle = \hat{T}(E^+) |\Phi_{\mathbf{a}}\rangle$$

...project:

$$\begin{aligned} \langle \Phi_{\mathbf{b}} | \hat{T}(E^+) | \Phi_{\mathbf{a}} \rangle &= \langle \Phi_{\mathbf{b}} | \hat{W} | \Psi_{\mathbf{a}}^{(+)} \rangle \\ &= -\frac{2\pi\hbar^2|A|^2}{\mu} f_{\mathbf{a},b}^{(+)}(\Omega_{kb}) \end{aligned}$$

$$\hat{G}_0(z) := [z - \hat{H}_0]^{-1}$$

$$[\mathbb{1} + \hat{G}\hat{W}] = [\mathbb{1} - \hat{G}_0\hat{W}]^{-1}$$

$$\hat{T}(z) = \hat{W} + \hat{W} \hat{G} \hat{W}$$

Formal Scattering

The Lippmann-Schwinger Equation

$$|\Psi_{\mathbf{a}}^{(+)}\rangle = [1 + \hat{G}(E^+) \hat{W}] |\Phi_{\mathbf{a}}\rangle$$

- This results in

$$f_{\mathbf{a},b}^{(+)}(\Omega_{kb}) = -\frac{\mu}{2\pi\hbar^2|A|^2} \langle \Phi_{\mathbf{b}} | \hat{T}(E^+) | \Phi_{\mathbf{a}} \rangle$$

- so that the scattering amplitude is (up to the numerical coefficients) the matrix element of the T-(transition)-operator.
- Given the iterative computation of the T-operator, this provides an iterative computation for the scattering amplitude:

$$\begin{aligned} f_{\mathbf{a},b}^{(+)}(\Omega_{kb}) = & -\frac{\mu}{2\pi\hbar^2|A|^2} \langle \Phi_{\mathbf{b}} | [\hat{W} + \hat{W}\hat{G}_0(E^+)\hat{W} \\ & + \hat{W}\hat{G}_0(E^+)\hat{W}\hat{G}_0(E^+)\hat{W} \\ & + \hat{W}\hat{G}_0(E^+)\hat{W}\hat{G}_0(E^+)\hat{W}\hat{G}_0(E^+)\hat{W} + \dots] | \end{aligned}$$

- ...and so on.
- This provides an iterative solution to the Lippmann-Schwinger equation and the scattering amplitude formally analogous to the stationary state perturbation expansion.

Formal Scattering

The T- and the S-Matrix

$$\begin{aligned} |\Psi_{\mathbf{a}}^{(+)}\rangle &= |\Phi_{\mathbf{a}}\rangle + \hat{G}_0(E^+) \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle \\ |\Psi_{\mathbf{a}}^{(+)}\rangle &= [\mathbb{1} + \hat{G}(E^+) \hat{W}] |\Phi_{\mathbf{a}}\rangle \end{aligned}$$

- The in- and the out-states are neither complete nor orthogonal
- Given $\hat{H} |\Psi_{\mathbf{a}}^{(+)}\rangle = E_a |\Psi_{\mathbf{a}}^{(+)}\rangle$ $\hat{H} |\Psi_{\mathbf{a}}^{(-)}\rangle = E_a |\Psi_{\mathbf{a}}^{(-)}\rangle$
- compute

$$\begin{aligned} \langle \Psi_{\mathbf{a}}^{(+)} | &= |\Psi_{\mathbf{a}}^{(+)}\rangle^\dagger = \left([\mathbb{1} + \hat{G}(E_a + i\epsilon) \hat{W}] |\Phi_{\mathbf{a}}\rangle \right)^\dagger = \langle \Phi_{\mathbf{a}} | [\mathbb{1} + \hat{G}(E_a + i\epsilon) \hat{W}]^\dagger \\ &= \langle \Phi_{\mathbf{a}} | [\mathbb{1} + \hat{W} \hat{G}(E_a - i\epsilon)] \end{aligned}$$

$$\langle \Psi_{\mathbf{a}}^{(+)} | \Psi_{\mathbf{b}}^{(+)} \rangle = \langle \Phi_{\mathbf{a}} | [\mathbb{1} + \hat{W} \hat{G}(E_a - i\epsilon)] | \Psi_{\mathbf{b}}^{(+)} \rangle$$

Formal Scattering

The T- and the S-Matrix

$$\begin{aligned} |\Psi_a^{(+)}\rangle &= |\Phi_a\rangle + \hat{G}_0(E^+) \hat{W} |\Psi_a^{(+)}\rangle \\ |\Psi_a^{(+)}\rangle &= [1 + \hat{G}(E^+) \hat{W}] |\Phi_a\rangle \end{aligned}$$

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Given $\hat{H} |\Psi_a^{(+)}\rangle = E_a |\Psi_a^{(+)}\rangle \quad \hat{H} |\Psi_a^{(-)}\rangle = E_a |\Psi_a^{(-)}\rangle$

• compute

$$\begin{aligned} \langle \Psi_a^{(+)} | &= |\Psi_a^{(+)}\rangle^\dagger = \left([1 + \hat{G}(E_a + i\epsilon) \hat{W}] |\Phi_a\rangle \right)^\dagger = \langle \Phi_a | [1 + \hat{G}(E_a + i\epsilon) \hat{W}]^\dagger \\ &= \langle \Phi_a | [1 + \hat{W} \hat{G}(E_a - i\epsilon)] \end{aligned}$$

$$\begin{aligned} \langle \Psi_a^{(+)} | \Psi_b^{(+)} \rangle &= \langle \Phi_a | [1 + \hat{W} \hat{G}(E_a - i\epsilon)] |\Psi_b^{(+)}\rangle \\ &= \langle \Phi_a | \Psi_b^{(+)} \rangle + \langle \Phi_a | \hat{W} [E_a - i\epsilon - \hat{H}]^{-1} |\Psi_b^{(+)}\rangle \\ &= \langle \Phi_a | \left(|\Phi_b\rangle + [E_b + i\epsilon - \hat{H}_0]^{-1} \hat{W} |\Psi_b^{(+)}\rangle \right) \\ &\quad + \langle \Phi_a | \hat{W} [E_a - i\epsilon - E_b]^{-1} |\Psi_b^{(+)}\rangle \end{aligned}$$

Formal Scattering

The T- and the S-Matrix

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$$\begin{aligned} \langle \Psi_a^{(+)} | &= |\Psi_a^{(+)}\rangle^\dagger = \left([\mathbb{1} + \hat{G}(E_a+i\epsilon) \hat{W}] |\Phi_a\rangle \right)^\dagger = \langle \Phi_a | [\mathbb{1} + \hat{G}(E_a+i\epsilon) \hat{W}]^\dagger \\ &= \langle \Phi_a | [\mathbb{1} + \hat{W} \hat{G}(E_a-i\epsilon)] \end{aligned}$$

$$\begin{aligned} \langle \Psi_a^{(+)} | \Psi_b^{(+)} \rangle &= \langle \Phi_a | [\mathbb{1} + \hat{W} \hat{G}(E_a-i\epsilon)] |\Psi_b^{(+)}\rangle \\ &= \langle \Phi_a | \Psi_b^{(+)} \rangle + \langle \Phi_a | \hat{W} [E_a - i\epsilon - \hat{H}]^{-1} |\Psi_b^{(+)}\rangle \\ &= \langle \Phi_a | \left(|\Phi_b\rangle + [E_b + i\epsilon - \hat{H}_0]^{-1} \hat{W} \right) |\Psi_b^{(+)}\rangle \\ &\quad + \langle \Phi_a | \hat{W} [E_a - i\epsilon - E_b]^{-1} |\Psi_b^{(+)}\rangle \\ &= \langle \Phi_a | \Phi_b \rangle + \langle \Phi_a | [E_b + i\epsilon - E_a]^{-1} \hat{W} |\Psi_b^{(+)}\rangle \\ &\quad + \langle \Phi_a | \hat{W} [E_a - i\epsilon - E_b]^{-1} |\Psi_b^{(+)}\rangle \end{aligned}$$

Formal Scattering

The T- and the S-Matrix

$$\begin{aligned} |\Psi_{\mathbf{a}}^{(+)}\rangle &= |\Phi_{\mathbf{a}}\rangle + \hat{G}_0(E^+) \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle \\ |\Psi_{\mathbf{a}}^{(+)}\rangle &= [\mathbb{1} + \hat{G}(E^+) \hat{W}] |\Phi_{\mathbf{a}}\rangle \end{aligned}$$

- The in- and the out-states are neither complete nor orthogonal

Given $\hat{H} |\Psi_{\mathbf{a}}^{(+)}\rangle = E_a |\Psi_{\mathbf{a}}^{(+)}\rangle \quad \hat{H} |\Psi_{\mathbf{a}}^{(-)}\rangle = E_a |\Psi_{\mathbf{a}}^{(-)}\rangle$

- compute

$$\begin{aligned} \langle \Psi_{\mathbf{a}}^{(+)} | &= |\Psi_{\mathbf{a}}^{(+)}\rangle^\dagger = \left([\mathbb{1} + \hat{G}(E_a + i\epsilon) \hat{W}] |\Phi_{\mathbf{a}}\rangle \right)^\dagger = \langle \Phi_{\mathbf{a}} | [\mathbb{1} + \hat{G}(E_a + i\epsilon) \hat{W}]^\dagger \\ &= \langle \Phi_{\mathbf{a}} | [\mathbb{1} + \hat{W} \hat{G}(E_a - i\epsilon)] \end{aligned}$$

$$\langle \Psi_{\mathbf{a}}^{(+)} | \Psi_{\mathbf{b}}^{(+)} \rangle = \langle \Phi_{\mathbf{a}} | \Phi_{\mathbf{b}} \rangle + \frac{\cancel{\langle \Phi_{\mathbf{a}} | \hat{W} | \Psi_{\mathbf{b}}^{(+)} \rangle}}{E_b + i\epsilon - E_a} + \frac{\cancel{\langle \Phi_{\mathbf{a}} | \hat{W} | \Psi_{\mathbf{b}}^{(+)} \rangle}}{E_a - i\epsilon - E_b}$$

$$= \langle \Phi_{\mathbf{a}} | \Phi_{\mathbf{b}} \rangle = (2\pi)^3 \delta^{(3)}(\vec{k}_a - \vec{k}_b) \delta_{a,b} \quad \text{orthogonal}$$

- Similarly

$$\langle \Psi_{\mathbf{a}}^{(-)} | \Psi_{\mathbf{b}}^{(-)} \rangle = \langle \Phi_{\mathbf{a}} | \Phi_{\mathbf{b}} \rangle = (2\pi)^3 \delta^{(3)}(\vec{k}_a - \vec{k}_b) \delta_{a,b} \quad \text{orthogonal}$$

Formal Scattering

The T- and the S-Matrix

$$\begin{aligned} |\Psi_a^{(+)}\rangle &= |\Phi_a\rangle + \hat{G}_0(E^+) \hat{W} |\Psi_a^{(+)}\rangle \\ |\Psi_a^{(+)}\rangle &= [\mathbb{1} + \hat{G}(E^+) \hat{W}] |\Phi_a\rangle \end{aligned}$$

- To prove the $^{+/-}$ non-orthogonality, calculate:

$$\begin{aligned} \langle \Psi_a^{(-)} | \Psi_b^{(+)} \rangle &= \langle \Phi_a | [\mathbb{1} + \hat{G}(E_a - i\epsilon) \hat{W}]^\dagger | \Psi_b^{(+)} \rangle \\ &= \langle \Phi_a | \Psi_b^{(+)} \rangle + \langle \Phi_a | \hat{W}[E_a + i\epsilon - \hat{H}]^{-1} | \Psi_b^{(+)} \rangle \\ &= \langle \Phi_a | \left(|\Phi_b\rangle + [E_b + i\epsilon - \hat{H}_0]^{-1} \hat{W} \right) | \Psi_b^{(+)} \rangle \\ &\quad + \langle \Phi_a | \hat{W}[E_a + i\epsilon - E_b]^{-1} | \Psi_b^{(+)} \rangle \\ &= \langle \Phi_a | \Phi_b \rangle + \langle \Phi_a | [E_b + i\epsilon - E_a]^{-1} \hat{W} | \Psi_b^{(+)} \rangle \\ &\quad + \langle \Phi_a | \hat{W}[E_a + i\epsilon - E_b]^{-1} | \Psi_b^{(+)} \rangle \\ &= \langle \Phi_a | \Phi_b \rangle + \frac{\langle \Phi_a | \hat{W} | \Psi_b^{(+)} \rangle}{E_b + i\epsilon - E_a} + \frac{\langle \Phi_a | \hat{W} | \Psi_b^{(+)} \rangle}{E_a + i\epsilon - E_b} \\ &= \langle \Phi_a | \Phi_b \rangle - \frac{2i\epsilon}{(E_a - E_b)^2 + \epsilon^2} \langle \Phi_a | \hat{W} | \Psi_b^{(+)} \rangle \\ &\xrightarrow{\epsilon \rightarrow 0} \langle \Phi_a | \Phi_b \rangle - 2\pi i \delta(E_a - E_b) \langle \Phi_a | \hat{W} | \Psi_b^{(+)} \rangle \end{aligned}$$

Formal Scattering

The T- and the S-Matrix

$$\begin{aligned} |\Psi_{\mathbf{a}}^{(+)}\rangle &= |\Phi_{\mathbf{a}}\rangle + \hat{G}_0(E^+) \hat{W} |\Psi_{\mathbf{a}}^{(+)}\rangle \\ |\Psi_{\mathbf{a}}^{(+)}\rangle &= [1 + \hat{G}(E^+) \hat{W}] |\Phi_{\mathbf{a}}\rangle \end{aligned}$$

Finally,

$$\langle \Psi_{\mathbf{a}}^{(-)} | \Psi_{\mathbf{b}}^{(+)} \rangle = (2\pi)^3 \delta^{(3)}(\vec{k}_a - \vec{k}_b) \delta_{a,b} - 2\pi i \delta(E_a - E_b) \langle \Phi_{\mathbf{a}} | \hat{T}(E_a^+) | \Phi_{\mathbf{b}} \rangle$$

Define:

$$\begin{aligned} S_{\mathbf{a},\mathbf{b}} &:= \langle \Psi_{\mathbf{a}}^{(-)} | \Psi_{\mathbf{b}}^{(+)} \rangle \\ &= (2\pi)^3 \delta^{(3)}(\vec{k}_a - \vec{k}_b) \delta_{a,b} - 2\pi i \delta(E_a - E_b) \hat{T}_{\mathbf{a},\mathbf{b}}(E_a^+) \end{aligned}$$

This S-matrix “translates” in-states into out-states:

$$\underbrace{|\Psi_{\mathbf{a}}^{(+)}\rangle}_{\text{out}} = \sum_{\mathbf{b}} \underbrace{|\Psi_{\mathbf{b}}^{(-)}\rangle}_{\text{in}} \underbrace{\langle \Psi_{\mathbf{b}}^{(-)} | \Psi_{\mathbf{a}}^{(+)} \rangle}_{S_{\mathbf{b},\mathbf{a}}} = \frac{1}{(2\pi)^3} \sum_b \int d^3 \vec{k}_b S_{\mathbf{b},\mathbf{a}} \underbrace{|\Psi_{\mathbf{b}}^{(-)}\rangle}_{\text{in}}$$

The δ -functions in the S-matrix insure that only states of the same energy are mixed (conservation of energy)

Formal Scattering

The T- and the S-Matrix

- The S -matrix is a unitary matrix:

$$|\Psi_{\mathbf{a}}^{(+)}\rangle = \sum_{\mathbf{b}} |\Psi_{\mathbf{b}}^{(-)}\rangle S_{\mathbf{b},\mathbf{a}} = \sum_{\mathbf{b}} |\Psi_{\mathbf{b}}^{(-)}\rangle \langle \Psi_{\mathbf{b}}^{(-)}| \Psi_{\mathbf{a}}^{(+)}\rangle$$

$$|\Psi_{\mathbf{b}}^{(-)}\rangle = \sum_{\mathbf{a}} |\Psi_{\mathbf{a}}^{(+)}\rangle \langle \Psi_{\mathbf{a}}^{(+)}| \Psi_{\mathbf{b}}^{(-)}\rangle = \sum_{\mathbf{a}} |\Psi_{\mathbf{a}}^{(+)}\rangle (S^{-1})_{\mathbf{a},\mathbf{b}}$$

$$(S^{-1})_{\mathbf{a},\mathbf{b}} = \langle \Psi_{\mathbf{a}}^{(+)}| \Psi_{\mathbf{b}}^{(-)}\rangle = (S_{\mathbf{b},\mathbf{a}})^* = (S^\dagger)_{\mathbf{a},\mathbf{b}}$$

- ...but it is not the matrix representation of a unitary operator!
- ...since scattering states do not form a complete basis.
- The S -matrix is only defined between states of the same energy:

$$S_{\mathbf{a},\mathbf{b}} = \delta_{\mathbf{a},\mathbf{b}} - 2\pi i \boxed{\delta(E_a - E_b)} T_{\mathbf{a},\mathbf{b}}(E_a^+) \quad \delta_{\mathbf{a},\mathbf{b}} = (2\pi)^3 \delta^3(\vec{k}_a - \vec{k}_b) \delta_{a,b}$$

- ...while the T-matrix is defined for all states:

$$\begin{aligned} T_{\mathbf{a},\mathbf{b}}(E) &= \langle \Phi_{\mathbf{a}} | \hat{T}(E) | \Phi_{\mathbf{b}} \rangle \\ &= \langle \Phi_{\mathbf{a}} | \hat{W} + \hat{G}_0 \hat{W} \hat{G}_0 + \hat{G}_0 \hat{W} \hat{G}_0 \hat{W} \hat{G}_0 + \dots | \Phi_{\mathbf{b}} \rangle \end{aligned}$$

Formal Scattering

The T- and the S-Matrix

- Unitarity of the S -matrix implies a condition for the T -matrix

$$\begin{aligned}\delta_{\mathbf{a},\mathbf{c}} &= (\mathbf{S}^\dagger)_{\mathbf{a},\mathbf{b}} S_{\mathbf{b},\mathbf{c}} = S_{\mathbf{b},\mathbf{a}}^* S_{\mathbf{b},\mathbf{c}} \\ &= [\delta_{\mathbf{b},\mathbf{a}} + 2\pi i \delta(E_b - E_a) T_{\mathbf{b},\mathbf{a}}^*] [\delta_{\mathbf{b},\mathbf{c}} - 2\pi i \delta(E_b - E_c) T_{\mathbf{b},\mathbf{c}}] \\ &= \delta_{\mathbf{a},\mathbf{c}} + 2\pi i \delta(E_c - E_a) [T_{\mathbf{c},\mathbf{a}}^* - T_{\mathbf{a},\mathbf{c}}] \\ &\quad + 4\pi^2 \sum_{\mathbf{b}} \delta(E_b - E_a) \delta(E_b - E_c) T_{\mathbf{b},\mathbf{a}}^* T_{\mathbf{b},\mathbf{c}}\end{aligned}$$

- Now,

$$\delta(E_b - E_a) \delta(E_b - E_c) = \delta(E_b - E_a) \delta(E_a - E_c)$$

Formal Scattering

The T- and the S-Matrix

- Unitarity of the S-matrix implies a condition for the T-matrix

$$\begin{aligned}
 \cancel{\delta_{\mathbf{a},\mathbf{c}}} &= (\mathbf{S}^\dagger)_{\mathbf{a},\mathbf{b}} S_{\mathbf{b},\mathbf{c}} = S_{\mathbf{b},\mathbf{a}}^* S_{\mathbf{b},\mathbf{c}} \\
 &= [\delta_{\mathbf{b},\mathbf{a}} + 2\pi i \delta(E_b - E_a) T_{\mathbf{b},\mathbf{a}}^*] [\delta_{\mathbf{b},\mathbf{c}} - 2\pi i \delta(E_b - E_c) T_{\mathbf{b},\mathbf{c}}] \\
 &= \cancel{\delta_{\mathbf{a},\mathbf{c}}} + 2\pi i \delta(E_c - E_a) [T_{\mathbf{c},\mathbf{a}}^* - T_{\mathbf{a},\mathbf{c}}] \\
 &\quad + 4\pi^2 \sum_{\mathbf{b}} \delta(E_b - E_a) \delta(E_b - E_c) T_{\mathbf{b},\mathbf{a}}^* T_{\mathbf{b},\mathbf{c}}
 \end{aligned}$$

Now,

$$\delta(E_b - E_a) \delta(E_b - E_c) = \delta(E_b - E_a) \delta(E_a - E_c) \quad \delta(E_c - E_a) = \delta(E_a - E_c)$$

so

$$0 = \frac{i}{2\pi} \cancel{\delta(E_a - E_c)} [T_{\mathbf{c},\mathbf{a}}^* - T_{\mathbf{a},\mathbf{c}}] + \sum_{\mathbf{b}} \delta(E_b - E_a) \cancel{\delta(E_a - E_c)} T_{\mathbf{b},\mathbf{a}}^* T_{\mathbf{b},\mathbf{c}}$$

i.e.,

$$\frac{1}{2\pi i} [T_{\mathbf{c},\mathbf{a}}^* - T_{\mathbf{a},\mathbf{c}}] = \sum_{\mathbf{b}} \delta(E_b - E_a) T_{\mathbf{b},\mathbf{a}}^* T_{\mathbf{b},\mathbf{c}}$$

Formal Scattering

$$T_{\mathbf{c},\mathbf{a}}(E_a^+) = -\frac{2\pi\hbar^2}{\mu} f_{\mathbf{a},c}^{(+)}(\Omega_{kc})$$

The T- and the S-Matrix

$$\frac{1}{2\pi i} [T_{\mathbf{c},\mathbf{a}}^* - T_{\mathbf{a},\mathbf{c}}] = \sum_{\mathbf{b}} \delta(E_b - E_a) T_{\mathbf{b},\mathbf{a}}^* T_{\mathbf{b},\mathbf{c}}$$

For $\mathbf{c} = \mathbf{a}$, this implies

$$\frac{1}{2\pi i} [T_{\mathbf{a},\mathbf{a}}^* - T_{\mathbf{a},\mathbf{a}}] = \sum_{\mathbf{b}} \delta(E_b - E_a) T_{\mathbf{b},\mathbf{a}}^* T_{\mathbf{b},\mathbf{a}}$$

$$-\frac{1}{\pi} \Im m[T_{\mathbf{a},\mathbf{a}}] = \frac{1}{(2\pi)^3} \sum_b \int d^3 \vec{k}_b \delta(E_b - E_a) |T_{\mathbf{b},\mathbf{a}}|^2$$

$$\frac{2\hbar^2}{\mu} \Im m[f_{\mathbf{a},a}(\theta=0)] = \frac{1}{(2\pi)^3} \sum_b \int k_b^2 dk_b \int d^2 \Omega_{kb} \delta\left(\frac{\hbar^2 k_b^2}{2\mu} - \frac{\hbar^2 k_a^2}{2\mu}\right) |T_{\mathbf{b},\mathbf{a}}|^2$$

forward
scattering
amplitude

$$= \frac{1}{(2\pi)^3} \sum_b \int k_b^2 dk_b \int d^2 \Omega_{kb} \frac{\mu}{\hbar^2 k_b} \delta(k_b - k_a) |T_{\mathbf{b},\mathbf{a}}|^2$$

$$= \frac{1}{(2\pi)^3} \frac{\mu}{\hbar^2} \sum_b k_b \int d^2 \Omega_{kb} |T_{\mathbf{b},\mathbf{a}}|^2$$

scattering probability
summed over all out-going states



Formal Scattering

The T- and the S-Matrix

- So, the unitarity of the S-matrix implies

$$\frac{2\hbar^2}{\mu} \Im m[f_{\mathbf{a},a}(\theta=0)] = \frac{1}{(2\pi)^3} \frac{\mu}{\hbar^2} \sum_b k_b \int d^2\Omega_{kb} |T_{\mathbf{b},\mathbf{a}}|^2$$

Now,

$$\begin{aligned} \sigma_T := \sigma_{\mathbf{a} \rightarrow \text{all}} &= \sum_{\substack{b \\ \text{all-inclusive}}} \int d^2\Omega_{kb} \sigma_{\mathbf{a} \rightarrow \mathbf{b}}(\Omega_{kb}) = \sum_b \int d^2\Omega_{kb} \frac{k_b}{k_a} |f_{\mathbf{a}\mathbf{b}}(\Omega_{kb})|^2 \\ &= \sum_b \int d^2\Omega_{kb} \frac{k_b}{k_a} \left| \frac{\mu}{2\pi\hbar^2} T_{\mathbf{b},\mathbf{a}} \right|^2 = \frac{\mu^2}{4\pi^2\hbar^4 k_a} \sum_b k_b \int d^2\Omega_{kb} |T_{\mathbf{b},\mathbf{a}}|^2 \end{aligned}$$

Formal Scattering

The T- and the S-Matrix

- So, the unitarity of the S-matrix implies

$$\frac{2\hbar^2}{\mu} \Im m[f_{\mathbf{a},a}(\theta=0)] = \frac{1}{(2\pi)^3} \frac{\mu}{\hbar^2} \sum_b k_b \int d^2\Omega_{kb} |T_{\mathbf{b},\mathbf{a}}|^2$$

Now,

$$\begin{aligned} \sigma_T := \sigma_{\mathbf{a} \rightarrow \text{all}} &= \sum_{\substack{b \\ \text{all-inclusive}}} \int d^2\Omega_{kb} \sigma_{\mathbf{a} \rightarrow \mathbf{b}}(\Omega_{kb}) = \sum_b \int d^2\Omega_{kb} \frac{k_b}{k_a} |f_{\mathbf{a}\mathbf{b}}(\Omega_{kb})|^2 \\ &= \sum_b \int d^2\Omega_{kb} \frac{k_b}{k_a} \left| \frac{\mu}{2\pi\hbar^2} T_{\mathbf{b},\mathbf{a}} \right|^2 = \frac{\mu^2}{4\pi^2\hbar^4 k_a} \sum_b k_b \int d^2\Omega_{kb} |T_{\mathbf{b},\mathbf{a}}|^2 \\ &= \frac{2\pi\mu}{\hbar^2 k_a} \boxed{\frac{1}{(2\pi)^3} \frac{\mu}{\hbar^2} \sum_b k_b \int d^2\Omega_{kb} |T_{\mathbf{b},\mathbf{a}}|^2} = \frac{2\pi\mu}{\hbar^2 k_a} \boxed{\frac{2\hbar^2}{\mu} \Im m[f_{\mathbf{a},a}(\theta=0)]} \end{aligned}$$

- Finally, we have:

$$\sigma_T = \frac{4\pi}{k_a} \Im m[f_{\mathbf{a},a}(\theta=0)]$$

optical theorem

Formal Scattering

The T- and the S-Matrix

- Using $S_{\mathbf{a},\mathbf{b}} := \langle \Psi_{\mathbf{a}}^{(-)} | \Psi_{\mathbf{b}}^{(+)} \rangle$ derive a few symmetry properties
- Time-reversal: $\hat{T} |\Psi_{\mathbf{a}}^{(+)}\rangle = |\Psi_{T\mathbf{a}}^{(-)}\rangle$ $T\mathbf{a} = \hat{T}(\vec{k}_a, a) = (-\vec{k}_a, Ta)$
- $\hat{T}(S_{\mathbf{b},\mathbf{a}}) = \hat{T}\langle \Psi_{\mathbf{b}}^{(-)} | \Psi_{\mathbf{a}}^{(+)} \rangle = \langle \Psi_{T\mathbf{b}}^{(+)} | \Psi_{T\mathbf{a}}^{(-)} \rangle = \langle \Psi_{T\mathbf{a}}^{(-)} | \Psi_{T\mathbf{b}}^{(+)} \rangle^* = S_{T\mathbf{a},T\mathbf{b}}^*$
- On the other hand, time-reversal is antilinear $\hat{T}(S_{\mathbf{b},\mathbf{a}}) = S_{\mathbf{b},\mathbf{a}}^*$
- This produces equalities among scattering amplitudes
- For cross-sections, $k_a^2 \sigma_{T\mathbf{a} \rightarrow T\mathbf{b}} = k_b^2 \sigma_{\mathbf{b} \rightarrow \mathbf{a}}$, from the bottom line
- If $(T\mathbf{a}, T\mathbf{b}) = (\mathbf{a}, \mathbf{b})$ up to 180°-rot (T-inv. int. states; e.g., no spin)

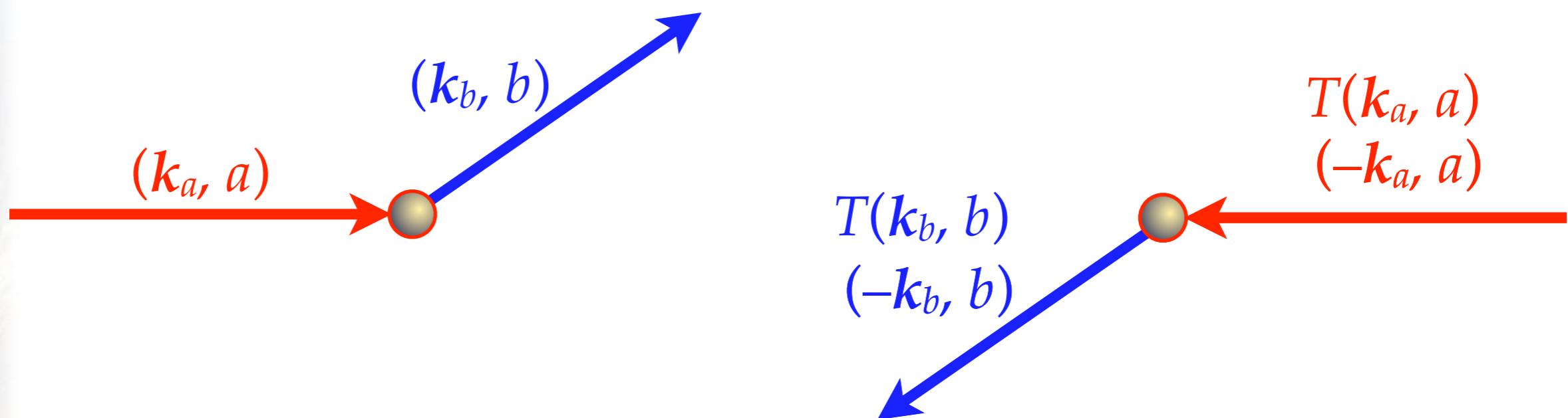
conjugation $\xrightarrow{*}$

$S_{T\mathbf{a},T\mathbf{b}}^*$	$=$	$\hat{T}(S_{\mathbf{b},\mathbf{a}})$	$=$	$S_{\mathbf{b},\mathbf{a}}^*$
\downarrow^*				\downarrow^*
$S_{T\mathbf{a},T\mathbf{b}}$	$=$	$\hat{T}(S_{\mathbf{b},\mathbf{a}}^*)$	$=$	$S_{\mathbf{b},\mathbf{a}}$

Formal Scattering

The T- and the S-Matrix

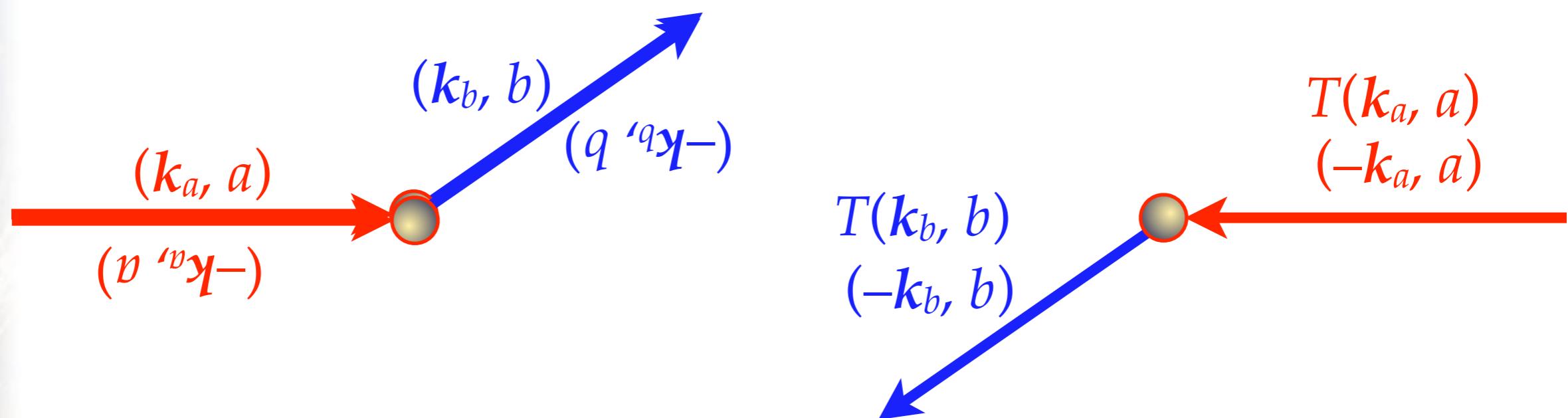
- If $(Ta, Tb) = (a, b)$ up to 180°-rot (T -inv. int. states; e.g., no spin)



Formal Scattering

The T- and the S-Matrix

- If $(T\mathbf{a}, T\mathbf{b}) = (\mathbf{a}, \mathbf{b})$ up to 180°-rot (T -inv. int. states; e.g., no spin)



Formal Scattering

The T- and the S-Matrix

- Using $S_{\mathbf{a},\mathbf{b}} := \langle \Psi_{\mathbf{a}}^{(-)} | \Psi_{\mathbf{b}}^{(+)} \rangle$ derive a few symmetry properties
- Time-reversal: $\hat{T} |\Psi_{\mathbf{a}}^{(+)}\rangle = |\Psi_{T\mathbf{a}}^{(-)}\rangle$ $T\mathbf{a} = \hat{T}(\vec{k}_a, a) = (-\vec{k}_a, Ta)$
- $\hat{T}(S_{\mathbf{b},\mathbf{a}}) = \hat{T}\langle \Psi_{\mathbf{b}}^{(-)} | \Psi_{\mathbf{a}}^{(+)} \rangle = \langle \Psi_{T\mathbf{b}}^{(+)} | \Psi_{T\mathbf{a}}^{(-)} \rangle = \langle \Psi_{T\mathbf{a}}^{(-)} | \Psi_{T\mathbf{b}}^{(+)} \rangle^* = S_{T\mathbf{a},T\mathbf{b}}^*$
- On the other hand, time-reversal is antilinear $\hat{T}(S_{\mathbf{b},\mathbf{a}}) = S_{\mathbf{b},\mathbf{a}}^*$
- This produces equalities among scattering amplitudes
- For cross-sections, $k_a^2 \sigma_{T\mathbf{a} \rightarrow T\mathbf{b}} = k_b^2 \sigma_{\mathbf{b} \rightarrow \mathbf{a}}$, from the bottom line
- If $(T\mathbf{a}, T\mathbf{b}) = (\mathbf{a}, \mathbf{b})$ up to 180°-rot (T-inv. int. states; e.g., no spin)
 - $(S_{T\mathbf{a},T\mathbf{b}} = S_{\mathbf{a},\mathbf{b}}) = S_{\mathbf{b},\mathbf{a}}$ the S-matrix is symmetric; detailed balance holds and reverse (inverse) scattering has the same scattering amplitude

conjugation $\xrightarrow{*}$

$S_{T\mathbf{a},T\mathbf{b}}^*$	$=$	$\hat{T}(S_{\mathbf{b},\mathbf{a}})$	$=$	$S_{\mathbf{b},\mathbf{a}}^*$
\downarrow^*				\downarrow^*
$S_{T\mathbf{a},T\mathbf{b}}$	$=$	$\hat{T}(S_{\mathbf{b},\mathbf{a}}^*)$	$=$	$S_{\mathbf{b},\mathbf{a}}$

Quantum Mechanics II

*Now, go forth and
calculate!!*

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