Scattering Theory

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Part I
Quantum Mechanics

This article is designed for leading the reader from old scattering theory of quantum mechanics to nowadays scattering theory of quantum field theory. The quantum mechanics part would be based on *Lectures on Quantum Mechanics* by S.Weinberg.

1 Potential Scattering

In this chapter we would study the theory of scattering in a simple but important case, the elastic scattering of a non-relativistic particle in a local potential, but using modern techniques that could easily be extended to more general problems.

1.1 In-States

Consider a non-relativistic particle of mass μ in a potential $V(\mathbf{x})$, whose Hamiltonian is,

$$H = H_0 + V(\mathbf{x}) \tag{1.1}$$

Here $H_0 = \mathbf{p}^2/2\mu$ is the kinetic energy operator. The potential is assumed to be function of position operator, and tends to zero as $|\mathbf{x}| = r \to \infty$. Then it is concerned here with a positive-energy particle[1]. The particle comes into facing the potential from great distances regarded to have no interaction with momentum $\hbar\mathbf{k}$, and is scattered, going out again to infinity, generally along a different direction.

In Heisenberg picture, for a particle with momentum $\hbar\mathbf{k}$ far from the scattering center if the measurement of the particle is made at very early times, and this situation is represented by a time-independent state vector $|\Psi_{\mathbf{k}}^{\text{in}}\rangle$. As mentioned, at very early times the particle is at a location that is far from the scattering center

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[1]Actually, there could possibly be negative energy if it is in bound state, that is, the energy is less than potential at boundaries. But now, we are considering scattering state, which is opposite with bound state.

so that the potential is negligible there, so the state has an energy $\hbar^2 \mathbf{k}^2/2\mu$, with the following relation,

$$H \ket{\Psi_{\mathbf{k}}^{\text{in}}} = \frac{\hbar^2 \mathbf{k}^2}{2\mu} \ket{\Psi_{\mathbf{k}}^{\text{in}}} \tag{1.2}$$

Now switch to Schrödinger picture, the state would evolve as time goes on. As mentioned, the scattering state would be continuous *superposition*[2] of states with a spread of energies,

$$\ket{\Psi_g(t)} = \int d^3k/(2\pi)^3\, g(\mathbf{k}) \exp\left(-i\frac{\hbar t \mathbf{k}^2}{2\mu}\right) \ket{\Psi_{\mathbf{k}}^{\text{in}}} \tag{1.3}$$

where $g(\mathbf{k})$ is a smooth function that is peaked around some wave number $\mathbf{k}_0$. The eigenstate $\ket{\Psi_{\mathbf{k}}^{\text{in}}}$ satisfies the further condition that for any sufficiently smooth function $g(\mathbf{k})$, in the limit $t \to -\infty$,

$$\ket{\Psi_g(t)} \to \int d^3k/(2\pi)^3\, g(\mathbf{k}) \exp\left(-i\frac{\hbar t \mathbf{k}^2}{2\mu}\right) \ket{\Phi_{\mathbf{k}}} \tag{1.4}$$

where $\ket{\Phi_{\mathbf{k}}}$ are orthonormal eigenstates of the momentum operator $\mathbf{P}$ with eigenvalue $\hbar\mathbf{k}$,

$$\mathbf{P}\ket{\Phi_{\mathbf{k}}} = \hbar\mathbf{k}\ket{\Phi_{\mathbf{k}}}$$
$$\braket{\Phi_{\mathbf{k}}|\Phi_{\mathbf{k}'}} = (2\pi)^3 \delta^{(3)}(\hbar\mathbf{k} - \hbar\mathbf{k}') \tag{1.5}$$

and hence eigenstates of H_0 (not H), with eigenvalue $E(|\mathbf{k}|) = \hbar^2 \mathbf{k}^2/2\mu$. Note that $\ket{\Psi_{\mathbf{k}}^{\text{in}}}$ and $\ket{\Phi_{\mathbf{k}}}$ belong to different Hilbert spaces. The incident wave packet $\ket{\Psi_g(t)}$ should satisfy the normalization condition $\braket{\Psi_g(t)|\Psi_g(t)} = 1$, which is equivalent to the condition at time limit,

$$\int\int d^3k\, d^3k'/(2\pi)^3\, g^*(\mathbf{k})g(\mathbf{k}') \exp\left(-i\frac{\hbar t}{2\mu}(\mathbf{k}'^2 - \mathbf{k}^2)\right) \delta^{(3)}(\hbar\mathbf{k} - \hbar\mathbf{k}')$$

$$= \hbar^{-3} \int d^3k/(2\pi)^3\, |g(\mathbf{k})|^2 = 1 \tag{1.6}$$

Rewrite the equation (1.2) as,

$$(E(|\mathbf{k}|) - H_0)\ket{\Psi_{\mathbf{k}}^{\text{in}}} = V\ket{\Psi_{\mathbf{k}}^{\text{in}}} \tag{1.7}$$

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[2]It would be discrete sum for a bound state.

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This has a formal solution,

$$|\Psi_{\mathbf{k}}^{\text{in}}\rangle = |\Phi_{\mathbf{k}}\rangle + (E(|\mathbf{k}|) - H_0 + i\epsilon)^{-1} |\Psi_{\mathbf{k}}^{\text{in}}\rangle \tag{1.8}$$

The first term on RHS could always be added up because it is the *homogeneous* solution of equation (1.7), and ϵ is a positive infinitesimal quantity, which is inserted to give meaning to the operator $(E(|\mathbf{k}|) - H_0 + i\epsilon)^{-1}$ when we integrate over the eigenvalues of H_0[3]. It is known as the *Lippmann-Schwinger equation*. The special feature of the particular 'solution' is that it also satisfies the additional initial condition.

To see this, we could expand $V |\Psi_{\mathbf{k}}^{\text{in}}\rangle$ in the orthonormal free-particle states $|\Phi_{\mathbf{q}}\rangle$:

$$V |\Psi_{\mathbf{k}}^{\text{in}}\rangle = \int d^3q/(2\pi)^3 |\Phi_{\mathbf{q}}\rangle \langle\Phi_{\mathbf{q}}| V |\Psi_{\mathbf{k}}^{\text{in}}\rangle \tag{1.9}$$

Thus equation (1.8) becomes,

$$|\Psi_{\mathbf{k}}^{\text{in}}\rangle = |\Phi_{\mathbf{k}}\rangle + \hbar^3 \int d^3q/(2\pi)^3 (E(|\mathbf{k}|) - H_0 + i\epsilon)^{-1} |\Phi_{\mathbf{q}}\rangle \langle\Phi_{\mathbf{q}}| V |\Psi_{\mathbf{k}}^{\text{in}}\rangle$$

$$= |\Phi_{\mathbf{k}}\rangle + \hbar^3 \int d^3q/(2\pi)^3 (E(|\mathbf{k}|) - E(|\mathbf{q}|) + i\epsilon)^{-1} |\Phi_{\mathbf{q}}\rangle \langle\Phi_{\mathbf{q}}| V |\Psi_{\mathbf{k}}^{\text{in}}\rangle \tag{1.10}$$

In calculating the integral over $\mathbf{k}$ in equation (1.3),

$$\int d^3k/(2\pi)^3 \, g(\mathbf{k}) \frac{\exp(-i\hbar t\mathbf{k}^2/2\mu)}{E(|\mathbf{k}|) - E(q) + i\epsilon} \langle\Phi_{\mathbf{q}}| V |\Psi_{\mathbf{k}}^{\text{in}}\rangle$$

$$= \int d\Omega \int_0^\infty dk/(2\pi)^3 \, k^2 g(\mathbf{k}) \frac{\exp(-i\hbar t\mathbf{k}^2/2\mu)}{E(k) - E(q) + i\epsilon} \langle\Phi_{\mathbf{q}}| V |\Psi_{\mathbf{k}}^{\text{in}}\rangle$$

where $d\Omega = \sin\theta \, d\theta d\phi$. We could convert the integral over k to an integral over the kinetic energy, using $dk = \mu dE/k\hbar^2$. Now, when $t \to -\infty$, the exponential term oscillates very rapidly, so that the only value of E that contribute are *those very near $E(q)$*, where the denominator also varies very rapidly.

$$= \int d\Omega/(2\pi)^3 \int_0^\infty dE \frac{\mu k}{\hbar^2} g(\mathbf{k}) \frac{\exp(-iEt/\hbar)}{E - E(q) + i\epsilon} \langle\Phi_{\mathbf{q}}| V |\Psi_{\mathbf{k}}^{\text{in}}\rangle$$

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[3]It is more reasonable in path integral formalism that the additional term must be added to prevent the integral diverges at large value of wave function.

Hence, for the time limit $t \to -\infty$, we could set $k = q$ everywhere except in the rapidly varying exponential and denominator,

$$= \int d\Omega/(2\pi)^3 \, g(\Omega) \frac{\mu q}{\hbar^2} \langle \Phi_\mathbf{q} | \, V \, | \Psi_\mathbf{q}^{\text{in}} \rangle \int_{\text{around E(q)}} dE \, \frac{\exp(-iEt/\hbar)}{E - E(q) + i\epsilon}$$

We could extend the integration range to the whole real axis, which is permissible because the integral receives no appreciable contributions anywhere that is far from $E(q)$,

$$\propto \int_{-\infty}^{\infty} dE \, \frac{\exp(-iEt/\hbar)}{E - E(q) + i\epsilon} \tag{1.11}$$

For $t \to -\infty$, we can close the contour of the integration with a very large semi-circle in the upper half of the complex plane, on which the integration is negligible because, for $\text{Im}(E) > 0$ and $t \to -\infty$, the numerator $\exp(-iEt/\hbar)$ is exponentially small. The only singularity of the integration is a pole at $E = E(q) - i\epsilon$, which is always in the lower half plane because ϵ is positive infinitesimal parameter. Hence, the integral vanishes for $t \to -\infty$. Only the first term of equation (1.10) is left, which gives the correct condition for $t \to -\infty$

1.2 Scattering Amplitudes

In the previous section, we defined a state that at early times has the appearance of a particle traveling toward a collision with a scattering center. Now we must consider what this state looks like after the collision.

For this purpose, we consider the coordinate-space wave function of the state $|\Psi_\mathbf{k}^{\text{in}}\rangle$[4].

$$V \, | \Psi_\mathbf{k}^{\text{in}} \rangle = \int d^3x \, | \Phi_\mathbf{x} \rangle \, \langle \Phi_\mathbf{x} | \, V \, | \Psi_\mathbf{k}^{\text{in}} \rangle = \int d^3x \, | \Phi_\mathbf{x} \rangle \, V(\mathbf{x}) \psi_\mathbf{k}(\mathbf{x}) \tag{1.12}$$

where $\psi_\mathbf{k}(\mathbf{x})$ is the coordinate-space wave function of the in-state,

$$\psi_\mathbf{k}(\mathbf{x}) = \langle \Phi_\mathbf{x} | \Psi_\mathbf{k}^{\text{in}} \rangle \tag{1.13}$$

Then, by taking the scalar product of the Lippmann-Schwinger equation (1.8), and using the fact that the scalar product of state of definite momentum and state of definite position would be plane-wave function,

$$\langle \Phi_\mathbf{x} | \Phi_\mathbf{k} \rangle = e^{i\mathbf{k} \cdot \mathbf{x}}$$

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[4]By this way, it would give us a physically vivid picture about scattering.

we have,

$$\psi_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \langle\Phi_{\mathbf{x}}| \left(E(|\mathbf{k}|) - H_0 + i\epsilon\right)^{-1} V |\Psi_{\mathbf{k}}^{\text{in}}\rangle$$

$$\psi_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \int d^3y \, \langle\Phi_{\mathbf{x}}| \left[E(|\mathbf{k}|) - H_0 + i\epsilon\right]^{-1} |\Phi_{\mathbf{y}}\rangle V(y)\psi_{\mathbf{k}}(\mathbf{y}) \quad (1.14)$$

where we define the Green function and then evaluate it by Fourier transform,

$$G_k(\mathbf{x} - \mathbf{y}) = \langle\Phi_{\mathbf{x}}| \left[E(|\mathbf{k}|) - H_0 + i\epsilon\right]^{-1} |\Phi_{\mathbf{y}}\rangle$$

$$= \int d^3q/(2\pi)^3 \, \frac{e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{y})}}{E(|\mathbf{k}|) - E(|\mathbf{q}|) + i\epsilon}$$

$$= \int -d\cos(\theta)d\phi \int q^2 dq/(2\pi)^3 \, \frac{e^{iq|\mathbf{x}-\mathbf{y}|\cos(\theta)}}{\hbar^2 k^2/2\mu - \hbar^2 q^2/2\mu + i\epsilon}$$

$$= \frac{2\pi}{(2\pi)^3} \int_0^\infty q^2 dq \, \frac{2i\sin(q|\mathbf{x}-\mathbf{y}|)}{iq|\mathbf{x}-\mathbf{y}|} \frac{2\mu/\hbar^2}{k^2 - q^2 + i\epsilon}$$

$$= -i\frac{2\mu}{\hbar^2} \frac{1}{4\pi^2|\mathbf{x}-\mathbf{y}|} \int_{-\infty}^\infty dq \, \frac{qe^{iq|\mathbf{x}-\mathbf{y}|}}{k^2 - q^2 + i\epsilon}$$

$$= -\frac{2\mu}{\hbar^2} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} e^{ik|\mathbf{x}-\mathbf{y}|} \quad (1.15)$$

The last line could be evaluated by completing the contour integral with a large semi-circle in the upper half plane. The poles are $q = \pm\sqrt{k^2 - i\epsilon} = k \pm i\epsilon$, and picking up the contribution of pole $q = k + i\epsilon$.

$$2\pi i \lim_{\epsilon\to 0} \frac{(k + i\epsilon)e^{i(k+i\epsilon)|\mathbf{x}-\mathbf{y}|}}{-(k + q + i\epsilon)} = -\pi i e^{ik|\mathbf{x}-\mathbf{y}|}$$

For a potential $V(\mathbf{y})$ that vanishes sufficiently rapidly as $|\mathbf{y}| \to \infty$. Write equation (1.14)

$$\psi_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \int d^3y \, G_{\mathbf{k}}(\mathbf{x} - \mathbf{y})V(\mathbf{y})\psi_{\mathbf{k}}(\mathbf{y}) \quad (1.16)$$

For $|\mathbf{x}| \to \infty$,

$$\psi_{\mathbf{k}}(\mathbf{x}) \to e^{i\mathbf{k}\cdot\mathbf{x}} + f_{\mathbf{k}}(\hat{x})e^{ikr}/r \quad (1.17)$$

where $|\mathbf{x}| \equiv r$ and $f_{\mathbf{k}}(\hat{x})$ is *scattering amplitude*.

$$f_{\mathbf{k}}(\hat{x}) = -\frac{\mu}{2\pi\hbar^2} \int d^3y \, e^{-ik\hat{x}\cdot\mathbf{y}} V(\mathbf{y})\psi_{\mathbf{k}}(\mathbf{y}) \quad (1.18)$$

There is an interesting result that the coordinate-space wave function would have incident-coming wave part and scattering wave part, and the scattering wave part would act like spherical wave.

Now let's consider how the superposition equation (1.3),

$$\psi_g(\mathbf{x}, t) \equiv \langle \Phi_\mathbf{x} | \Psi_g(t) \rangle = \int d^3k/(2\pi)^3 \, g(\mathbf{k}) \psi_\mathbf{k}(\mathbf{x}) \exp\left(-i\hbar t \mathbf{k}^2/2\mu\right) \quad (1.19)$$

in the limit $t \to +\infty$, with r/t held fixed, and $\mathbf{x}$ off the 3-axis[5], equation (1.19) gives[6],

$$\psi_g(\mathbf{x}, t) \to \frac{1}{(2\pi)^3 r} \int d^2 k_\perp \int_{-\infty}^{\infty} dk_3 \, g(\mathbf{k}_\perp, k_3)$$
$$\times \exp\left(ik_3 r - i\hbar t k_3^2/2\mu\right) f_{\mathbf{k}_0}(\hat{x}) \quad (1.20)$$

We have taken the subscript on the scattering amplitude to be $\mathbf{k}_0$, because the function g is sharply peaked at this value of $\mathbf{k}$, and we have approximated $k = \sqrt{k_3^2 + \mathbf{k}_\perp^2}$ as $k \approx k_3$ in the exponent, because $g(\mathbf{k}_\perp, k_3)$ is assumed to be negligible except for $|\mathbf{k}_\perp| << k_3$. That is, we assume that the function $g(\mathbf{k}_\perp, k_3)$, though smooth, is strongly peaked at $k_3 = k_0$ and $\mathbf{k}_\perp = 0$, so we could set k_3 in $g(\mathbf{k}_\perp, k_3)$ equal to the value $\mu r/\hbar t$, so that,

$$\psi_g(\mathbf{x}, t) \to \frac{1}{(2\pi)^3 r} f_{\mathbf{k}_0}(\hat{x}) \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu r/\hbar t)$$
$$\times \int_{-\infty}^{\infty} dk_3 \, \exp\left(ik_3 r - i\hbar t k_3^2/2\mu\right)$$
$$= \frac{1}{(2\pi)^3 r} f_{\mathbf{k}_0} \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu r/\hbar t) \exp\left(i\mu r^2/2\hbar t\right) \sqrt{\frac{2\pi\mu}{i\hbar t}} \quad (1.21)$$

Where we reach the last line by Gaussian integral.

The probability $dP(\hat{x})$ that the particle at late times is somewhere within the cone of infinitesimal solid angle $d\omega$ around the direction $\hat{x}$ is then the integral of $|\psi_g(\mathbf{x}, t)|^2$ over this cone:

$$dP(\hat{x}, \mathbf{k}_0) = d\Omega \int_0^{\infty} r^2 dr \, |\psi_g(\mathbf{x}, t)|^2 \quad (1.22)$$

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[5]Which means the first term in equation (1.17) vanishes.

[6]We would assume that the particle comes in from a great distance along the negative 3-axis, so we are interested in the limit of very large negative t and x_3, but with x_3/t held finite. And also assume the particle velocity is sufficiently closely confined to the 3-direction, where the function $g(\mathbf{k})$ is not negligible.

$$\to d\Omega \frac{2\mu\pi}{(2\pi)^6 \hbar t} |f_{\mathbf{k}_0}(\hat{x})|^2 \int_0^\infty dr \left| \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu r/\hbar t) \right|^2$$

changing the variable of integration r to $k_3 \equiv \mu r/\hbar t$,

$$\frac{d\,P(\hat{x}, \mathbf{k}_0)}{d\Omega} = |f_{\mathbf{k}_0}(\hat{x})|^2 \int_0^\infty dk_3/(2\pi)^5 \left| \int d^2 k_\perp \, g(\mathbf{k}_\perp, k_3) \right|^2 \tag{1.23}$$

Now, the coefficient of $|f_{\mathbf{k}_0}(\hat{x})|^2$ in equation (1.23) has the dimensions of an inverse area. In fact, it is precisely the probability per unit area that the particle is in a small area centered on the 3-axis and normal to that axis:

$$\rho_\perp \equiv \lim_{t\to-\infty} \int_{-\infty}^\infty dx_3 \, |\psi_g(0, x_3, t)|^2 \tag{1.24}$$

To see this, recall equation (1.4) and its scalar product with state of definite position,

$$\langle \Phi_{\mathbf{x}} | \Psi_g(t) \rangle \to \int d^3 k/(2\pi)^3 \, g(\mathbf{k}) \exp\left(i\mathbf{k} \cdot \mathbf{x} - i\hbar t k^2/2\mu\right)$$

As what we've done in equation (1.21), we assume that the particle moves along the 3-axis,

$$\langle \Phi_{\mathbf{x}} | \Psi_g(t) \rangle \to$$

$$\frac{1}{(2\pi)^3} \int d^2 k_\perp \int dk_3 \, g(\mathbf{k}_\perp, k_3) \exp\left(i\mathbf{k}_\perp \cdot \mathbf{x}_\perp + ik_3 x_3 - i\hbar t(k_3 - \mu x_3/\hbar t)^2/2\mu\right)$$

Replace k_3 with $k_3 = \mu x_3/\hbar t$ except the exponent term.

$$\langle \Phi_{\mathbf{x}} | \Psi_g(t) \rangle \to$$

$$\frac{1}{(2\pi)^3} \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu x_3/\hbar t) \exp(i\mathbf{k}_\perp \cdot \mathbf{x}_\perp)$$

$$\times \exp\left(ix_3^2 \mu/2\hbar t\right) \int_{-\infty}^\infty dk_3 \, \exp\left(-i\hbar t(k_3 - \mu x_3/\hbar t)^2/2\mu\right)$$

$$= \frac{1}{(2\pi)^3} \exp\left(ix_3^2 \mu/2\hbar t\right) \sqrt{\frac{2\mu\pi}{i\hbar t}} \times \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu x_3/\hbar t) \exp(i\mathbf{k}_\perp \cdot \mathbf{x}_\perp) \tag{1.25}$$

Therefore, in particular as t tends to infinity far (∞), the spatial probability distribution is,

$$|\langle \Phi_{\mathbf{x}} | \Psi_g(t) \rangle|^2 \to \frac{\mu}{\hbar t(2\pi)^5} \left| \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu x_3/\hbar t) \exp(i\mathbf{k}_\perp \cdot \mathbf{x}_\perp) \right|^2 \tag{1.26}$$

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Integrate over spatial with equation (1.26)[7],

$$\rho_\perp = \int dx_3 \, |\langle \Phi_{\mathbf{x}} | \Psi_g(t) \rangle|^2 \rightarrow \frac{\mu}{\hbar t (2\pi)^5} \int dx_3 \left| \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu x_3 / \hbar t) \right|^2$$

$$\rightarrow \frac{1}{(2\pi)^5} \int dk_3 \left| \int d^2 k_\perp \, g(\mathbf{k}_\perp, \mu x_3 / \hbar t) \right|^2$$

Hence, equation (1.23) may be written,

$$\frac{dP(\hat{x}, \mathbf{k}_0)}{d\Omega} = \rho_\perp \, |f_{\mathbf{k}_0}(\hat{x})|^2 \tag{1.27}$$

We define the *differential cross-section* as the ratio,

$$\frac{d\sigma(\hat{x}, \mathbf{k}_0)}{d\Omega} \equiv \frac{1}{\rho_\perp} \frac{dP(\hat{x}, \mathbf{k}_0)}{d\Omega} = |f_{\mathbf{k}_0}(\hat{x})|^2 \tag{1.28}$$

We could think of $d\sigma(\hat{x}, \mathbf{k}_0)$ as a tiny area normal to the 3-axis, where the incoming particle must hit in order for it to be scattered into a solid angle $d\Omega$ around the direction $\hat{x}$. The equation (1.28) then says that the probability of the above process to happen equals the ratio of $d\omega$ to the effective cross-sectional area $1/\rho_\perp$ of the beam.

Of course, to measure $d\sigma/d\Omega$, experimenters do not actually send a particle or particles toward a single target. Instead, they direct a beam of particles toward a thin slab containing some large number N_T of targets. Scattering into some particular range of angles can occur only if a particle from the beam hits a tiny area $d\sigma$ around one of the targets, then the number of particles that are scattered into this range of angles[8] is the number of beam particles per unit transverse area $\mathcal{N}_B$, times the total area $N_T d\sigma$ that the beam particles have to hit upon.

2 General Scattering Theory

There are much more general circumstances to which scattering theory is applicable. The scattering can produce additional particles; the interaction may not be a local potential; some or all of the particles involved may be moving at relativistic velocities; some may be photon (massless); and the initial state may even contain more than two particles. This section would describe scattering theory at a level of generality that encompasses all these possibilities.

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[7]Note that we only integrate over 3-axis, so the dimension is the probability per unit area.

[8]Or says, the number of scattering event.

2.1 The S-Matrix

We again assume that the Hamiltonian H is the sum of an unperturbed Hermitian (free Hamiltonian) term H_0, describing any number of non-interacting particles, plus some sort of interaction V:

$$H = H_0 + V \tag{2.1}$$

The only assumptions we make about V are that it is Hermitian, and that its effects become negligible when the particles described by H_0 are fall from one another[9].

In section 1.1 we defined an "in" state $|\Psi_{\mathbf{k}}^{\text{in}}\rangle$ as an eigenstate of the Hamiltonian H that looks like it consists of a single particle with momentum $\hbar\mathbf{k}$ far from the scattering center if measurements are made at sufficiently early times. We generalize this definition, and define "in" and "out" state $|\Psi_\alpha^+\rangle$ and $|\Psi_\alpha^-\rangle$ as eigenstates of the Hamiltonian

$$H|\Psi_\alpha^\pm\rangle = E_\alpha |\Psi_\alpha^\pm\rangle \tag{2.2}$$

and both look like an eigenstate Φ_α of the free-particle Hamiltonian

$$H_0|\Phi_\alpha\rangle = E_\alpha|\Phi_\alpha\rangle \tag{2.3}$$

The states consist of a number of particles at great distances from each other[10], provided measurements are made at very early times (for $|\Psi_\alpha^+\rangle$) or very late times (for $|\Psi_\alpha^-\rangle$). Here α is a compound index, standing for the types and numbers of the particles in the state, as well as their momenta and spin 3-componets (or helicities). It will be convenient to choose the states $|\Phi_\alpha\rangle$ to be orthonormal

$$\langle\Phi_\beta|\Phi_\alpha\rangle = \delta(\beta - \alpha) \tag{2.4}$$

The ambiguous delta function $\delta(\alpha - \beta)$ consists of a product of Kronecher deltas for the numbers and types and spin 3-componets of corresponding particles in the states α and β, together with 3-dimensional delta functions for the momenta of the corresponding particles in these states.

The definition of $|\Psi_\alpha^+\rangle$ and $|\Psi_\alpha^-\rangle$ can be made more precise by specifying that if $g(\alpha)$ **is a sufficiently smooth function of the momenta** in the state α, then (as a generalization of equation (1.4))

$$\int d\alpha\, g(\alpha) \exp(-iE_\alpha t/\hbar)|\Psi_\alpha^\pm\rangle \to \int d\alpha\, g(\alpha) \exp\{-iE_\alpha t/\hbar\}|\Phi_\alpha\rangle \tag{2.5}$$

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[9]Neither scattering center nor local potential are considered in general scattering theory.

[10]Where the effects of interaction are negligible.

for $t \to \mp\infty$. (Ambiguously integrals over α include sums over the numbers and types of particles along with the 3-components of their spins, as well as integrals over the momenta of all the particles in the state α.) We could satisfy this condition by rewriting equation (2.5) as a generalization of the Lippmann-Schwinger equation (1.8):

$$\Psi_\alpha^\pm = \Phi_\alpha + (E_\alpha - H_0 \pm i\epsilon)^{-1} V \Psi_\alpha^\pm \tag{2.6}$$

with ϵ is positive infinitesimal parameter. Equation (2.5) then follows by a simple extension of the argument used in Section 1.1. From equation (2.6) we can verify the further condition (equation (2.5)) of superposition of plane wave

$$\int d\alpha\, g(\alpha) \exp(-iE_\alpha t/\hbar) \, |\Psi_\alpha^\pm\rangle = \int d\alpha\, g(\alpha) \exp(-iE_\alpha t/\hbar) \, |\Phi_\alpha\rangle$$

$$+ \int d\alpha \int d\beta \, \frac{g(\alpha) \exp(-iE_\alpha t/\hbar) \langle\Phi_\beta| V \, |\Psi_\alpha^\pm\rangle}{E_\alpha - E_\beta \pm i\epsilon} \, |\Phi_\beta\rangle \tag{2.7}$$

[11] The rapid oscillation of the exponential in the second term on the right-hand side kills all contributions to this integral except those from E_α near E_β, where the denominator also varies rapidly. In particular, as we did in Section 1.1, this allows us to extend the integral to all real E_α[12], because no part of the range of integration except very near E_β will contribute as $|t| \to \infty$. This integral can be evaluated for $|t| \to \infty$ by closing the contour of integration over E_α with a large semicircle in the upper half of the complex plane for $t \to -\infty$ or in the lower half of the complex plane for $t \to \infty$, because in both case the factor $\exp(-iE_\alpha t/\hbar)$ is exponentially damped on the semicircle due to the positive (negative) imagery part of E_α. In both cases the pole at $E_\alpha = E_\beta \mp i\epsilon$ is outside the contour of integration, so this integral vanishes, leaving us with equation (2.5).

The "in" and "out" states inhabit the same Hilbert space, and are distinguished only by how they are described, by their appearance at $t \to -\infty$ or at $t \to \infty$. Indeed, any "in" state can be expressed as a superposition of "out" states:

$$|\Psi_\alpha^+\rangle = \int d\beta \, S_{\beta\alpha} \, |\Psi_\beta^-\rangle \tag{2.8}$$

The coefficient $S_{\alpha\beta}$ in this relation form is known as the *S-matrix*. If we arrange a state so that it appears at $t \to -\infty$ like a free-particle state $|\Phi_\alpha\rangle$, then the state

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[11]We integrate over β so that the free-particle operator H_0 would become eigenvalue E_β.

[12]Because $d\alpha$, as mentioned before, represents the integration over the momenta of all the particles in the state α, which can be easily changed to integral over the energy by energy-momentum relation.

is $|\Psi_\alpha^+\rangle$, and equation (2.8) tells us that the state will appear at late times like the superposition $\int d\beta\, S_{\beta\alpha}\,|\Phi_\beta\rangle$. As we will see, the S-matrix contains all information about the rates of reactions among particles of any sort.

We can derive a useful formula for the S-matrix by considering what the "in" state looks like if measurements are made at *late* times. We again use equation (2.7) for $|\Psi_\alpha^+\rangle$, but now because $t > 0$ we can only close the contour of integration of E_α in the second term with a large semicircle in the *lower* half of the complex plane, so now we receive a contribution from the pole at $E_\alpha = E_\beta - i\epsilon$[13]. Because we are integrating over a closed contour running in the *clockwise* direction, the contribution of this pole is $-2\pi i$ times the same integral, but with the denominator dropped, and with the integration over E_α replaced by setting $E_\alpha = E_\beta - i\epsilon$ in the remainder of the integral. Because ϵ is infinitesimal positive, this is just amounts to replacing $(E_\alpha - E_\beta + i\epsilon)^{-1}$ in equation (2.7) with $-2\pi i\delta(E_\alpha - E_\beta)$, so that for $t \to +\infty$

$$\int d\alpha\, g(\alpha) \exp(-iE_\alpha t/\hbar)\,|\Psi_\alpha^+\rangle \to \int d\alpha\, g(\alpha) \exp(-iE_\alpha t/\hbar)\,|\Phi_\alpha\rangle$$

$$-2\pi i \int d\alpha \int d\beta\, g(\alpha) \exp(-iE_\alpha t/\hbar)\,\langle\Phi_\beta|\,V\,|\Psi_\alpha^+\rangle\,\delta(E_\alpha - E_\beta)\,|\Phi_\beta\rangle \qquad (2.9)$$

As mentioned previously, the state $|\Psi_\alpha^+\rangle$ would, at $t \to -\infty$, look like the superposition $\int d\beta\, S_{\beta\alpha}\,|\Phi_\beta\rangle$, so from equation (2.9), we have,

$$S_{\beta\alpha} = \delta(\beta - \alpha) - 2\pi i\delta(E_\alpha - E_\beta)T_{\beta\alpha} \qquad (2.10)$$

where

$$T_{\beta\alpha} \equiv \langle\Phi_\beta|\,V\,|\Psi_\alpha^+\rangle \qquad (2.11)$$

By taking the scalar product of equation (2.8) with $\langle\Psi_\beta^-|$

$$\langle\Psi_\beta^-|\Psi_\alpha^+\rangle = \int d\gamma\, S_{\gamma\alpha}\,\langle\Psi_\beta^-|\Psi_\gamma^-\rangle$$

$$= \int d\gamma\, S_{\gamma\alpha}\delta(\beta - \gamma)$$

$$= S_{\beta\alpha} \qquad (2.12)$$

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[13]Because the pole is at the lower half of the complex plane.

Thus $S_{\beta\alpha}$ is the probability amplitude that a state that is arranged to look like the free-particle state $|\Phi_\alpha\rangle$ at $t \to -\infty$ and would look like the free-particle state $|\Phi_\beta\rangle$ when measurements are made at $t \to \infty$.

<center>* * *</center>

We have chosen the free-particles states $|\Phi_\alpha\rangle$ to be orthonormal, and it follows then from equation (2.6) that the "in" and "out" states are also orthonormal. This is fairly obvious from the condition (2.5), but there is also a more direct proof. We can evaluate the matrix element $\langle \Psi_{\beta\pm}| V |\Psi_\alpha^\pm\rangle$ by using equation (2.6) in either the right or left side of the scalar product. Using the fact that H_0 and V are Hermitian, the results must be equal applying operators on either bra or ket

$$\langle \Psi_\beta^\pm| V |\Phi_\alpha\rangle + \langle \Psi_\beta^\pm| V (E_\alpha - H_0 \pm i\epsilon)^{-1} V |\Psi_\alpha^\pm\rangle =$$

$$\langle \Phi_\beta| V |\Psi_\alpha^\pm\rangle + \langle \Psi_\beta^\pm| V (E_\beta - H_0 \mp i\epsilon)^{-1} V |\Psi_\alpha^\pm\rangle \tag{2.13}$$

Also, we have the following identity

$$\frac{1}{E_\alpha - H_0 \pm i\epsilon} - \frac{1}{E_\beta - H_0 \mp i\epsilon} =$$

$$\frac{E_\alpha - H_0 \pm i\epsilon - E_\beta + H_0 \pm i\epsilon}{(E_\alpha - H_0 \pm i\epsilon)(E_\beta - H_0 \mp i\epsilon)} =$$

$$\frac{E_\alpha - E_\beta \pm 2i\epsilon}{(E_\alpha - H_0 \pm i\epsilon)(E_\beta - H_0 \mp i\epsilon)} \tag{2.14}$$

then divide the equation (2.13) by $E_\alpha - E_\beta \pm 2i\epsilon$

$$\frac{\langle \Psi_\beta^\pm| V |\Phi_\alpha\rangle}{E_\alpha - E_\beta \pm 2i\epsilon} - \frac{\langle \Phi_\beta| V |\Psi_\alpha^\pm\rangle}{E_\alpha - E_\beta \pm 2i\epsilon}$$

$$= \frac{\langle \Psi_\beta^\pm| V (E_\alpha - H_0 \pm i\epsilon)^{-1} V |\Psi_\alpha^\pm\rangle - \langle \Psi_\beta^\pm| V (E_\beta - H_0 \mp i\epsilon)^{-1} |\Psi_\alpha^\pm\rangle}{E_\alpha - E_\beta \pm 2i\epsilon}$$

$$= \langle \Psi_\beta^\pm| V (E_\beta - H_0 \mp i\epsilon)^{-1} (E_\alpha - H_0 \pm i\epsilon)^{-1} V |\Psi_\alpha^\pm\rangle \tag{2.15}$$

further simplify LHS, because the only important thing about ϵ is that it is a positive infinitesimal, so we may as well replace 2ϵ here with ϵ.

$$- \left(\langle \Phi_\alpha| (E_\beta - H_0 \pm i\epsilon)^{-1} V |\Psi_\beta^\pm\rangle \right)^* - \langle \Phi_\beta| (E_\alpha - H_0 \pm i\epsilon)^{-1} V |\Psi_\alpha^\pm\rangle$$

$$= \langle \Psi_\beta^\pm| V (E_\beta - H_0 \mp i\epsilon)^{-1} (E_\alpha - H_0 \pm i\epsilon)^{-1} V |\Psi_\alpha^\pm\rangle \tag{2.16}$$

<center>13</center>

according to equation (2.6), this tells us,

$$-(\langle\Phi_\alpha|\Psi_\beta^\pm - \Phi_\beta\rangle)^* - \langle\Phi_\beta|\Psi_\alpha^\pm - \Phi_\alpha\rangle = \langle\Psi_\beta^\pm - \Phi_\beta|\Psi_\alpha^\pm - \Phi_\alpha\rangle \qquad (2.17)$$

and therefore

$$\langle\Psi_\beta^\pm|\Psi_\alpha^\pm\rangle = \langle\Phi_\beta|\Phi_\alpha\rangle = \delta(\beta - \alpha) \qquad (2.18)$$

Because $S_{\beta\alpha}$ is the matrix of the scalar products of two complete orthonormal sets of state vectors, it must be unitary. We can also show this directly by multiplying equation (2.13) (for "in" states) with $\delta(E_\alpha - E_\beta)$, from which we learn that, recall

$$T_{\beta\alpha} = \langle\Phi_\beta|V|\Psi_\alpha^+\rangle$$

so that

$$\left(\langle\Phi_\alpha|V|\Psi_\beta^+\rangle\right)^* - \langle\Phi_\beta|V|\Psi_\alpha^+\rangle = \langle\Psi_\beta^+|V(E_\beta - H_0 - i\epsilon)^{-1}V|\Psi_\alpha^+\rangle$$

$$- \langle\Psi_\beta^+|V(E_\alpha - H_0 + i\epsilon)^{-1}V|\Psi_\alpha^+\rangle$$

expand the RHS with complete free-particle state,

$$T_{\alpha\beta}^* - T_{\beta\alpha} = (E_\alpha - E_\beta + 2i\epsilon)$$

$$\int d\gamma \left[\langle\Psi_\beta^+|V(E_\beta - E_\gamma - i\epsilon)^{-1}|\Phi_\gamma\rangle \langle\Phi_\gamma|(E_\alpha - E_\gamma + i\epsilon)^{-1}V|\Psi_\alpha^+\rangle\right]$$

now multiply the whole thing with the delta function and simplify the RHS,

$$\delta(E_\alpha - E_\beta)\left(T_{\alpha\beta}^* - T_{\beta\alpha}\right) = 2i\epsilon\delta(E_\alpha - E_\beta)\int d\gamma \frac{T_{\gamma\beta}^* T_{\gamma\alpha}}{(E_\alpha - E_\gamma)^2 + \epsilon^2}$$

Consider the integral over E_γ, and for infinitesimal ϵ, the function $\epsilon/(x^2 + \epsilon^2)$ is negligible away from $x = 0$, with its integral over all x ($\int dx\, \epsilon/(x^2 + \epsilon^2)$) being π[14].

$$2i\epsilon\delta(E_\alpha - E_\beta)\int d\gamma\, T_{\gamma\beta}^* T_{\gamma\alpha} \cdot \pi\delta(E_\alpha - E_\gamma)$$

Multiplying with $-2i\pi$

$$-2i\pi\delta(E_\alpha - E_\beta)(T_{\alpha\beta}^* - T_{\beta\alpha}) =$$

$$\int d\gamma \left[2i\pi\delta(E_\gamma - E_\beta)T_{\gamma\beta}^*\right]\left[-2i\pi\delta(E_\gamma - E_\alpha)T_{\gamma\alpha}\right]$$

---

[14]Using trigonometric substitution, and integral over E_γ considering $E_\gamma = E_\alpha$ in the numerator.

and recalling equation (2.10)

$$- [S_{\beta\alpha} - \delta(\alpha - \beta)] - [S_{\alpha\beta} - \delta(\beta - \alpha)]^*$$

$$= \int d\gamma \; [S_{\gamma\beta} - \delta(\gamma - \beta)]^* \, [S_{\gamma\alpha} - \delta(\gamma - \alpha)] \qquad (2.19)$$

expand the braket,

$$-S_{\beta\alpha} + \delta(\alpha - \beta) - S_{\alpha\beta}^* + \delta(\beta - \alpha) =$$

$$\int d\gamma \; \left[-S_{\gamma\beta}^* \delta(\gamma - \alpha) - \delta(\gamma - \beta) S_{\gamma\alpha} + S_{\gamma\beta}^* S_{\gamma\alpha} + \delta(\gamma - \beta)\delta(\gamma - \alpha) \right]$$

the RHS would be

$$-S_{\alpha\beta}^* - S_{\beta\alpha} + \int d\gamma \, S_{\gamma\beta}^* S_{\gamma\alpha} + \delta(\beta - \alpha)$$

or in other words

$$\int d\gamma \, S_{\gamma\beta}^* S_{\gamma\alpha} = \delta(\alpha - \beta) \qquad (2.20)$$

which says S-matrix is unitary.

2.2 Rates

$\hbar$ is set to unity.

The S-matrix given by equation (2.10) evidently conserves energy[15]. More importantly, the symmetry of invariance under spatial translations[16] tells us that $T_{\beta\alpha}$ and $S_{\beta\alpha}$ are proportional to a three-dimensional delta function $\delta^{(3)}(\mathbf{P}_\alpha - \mathbf{P}_\beta)$, where $\mathbf{P}_\alpha$ and $\mathbf{P}_\beta$ are the total momenta of the states α and β. In the case where α and β are not identical states, we can write

$$S_{\beta\alpha} = \delta(E_\alpha - E_\beta)\delta^{(3)}(\mathbf{P}_\alpha - \mathbf{P}_\beta)M_{\beta\alpha} \qquad (2.21)$$

where $M_{\beta\alpha}$ is a smooth function of the momenta in the states α and β. The presence of the delta functions in equation (2.21) poses an immediate problem: in setting the probability for the transition $\alpha \to \beta$ equal to $|S_{\beta\alpha}|^2$, what are we to make of the squares of delta functions?

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[15]There are $\delta(E_\alpha - E_\beta)$ in both the first term and the second term.

[16]Because it is assumed no fixed scattering center in the general scattering theory.

The easiest way to deal with this problem is to imagine that the system is contained in a box of finite volume V, and that the interaction is turned on only for a finite time T. One consequence is that the delta functions are instead replaced with,

$$\delta_V^{(3)}(\mathbf{P}_\alpha - \mathbf{P}_\beta) \equiv \frac{1}{(2\pi)^3} \int_V d^3x \, e^{i(\mathbf{P}_\alpha - \mathbf{P}_\beta)\cdot\mathbf{x}}$$

$$\delta_T(E_\alpha - E_\beta) \equiv \frac{1}{2\pi} \int_T dt \, e^{i(E_\alpha - E_\beta)t} \tag{2.22}$$

Hence, the square of delta functions would be

$$\left[\delta_V^{(3)}(\mathbf{P}_\alpha - \mathbf{P}_\beta)\right]^2 = \frac{V}{(2\pi)^3} \delta_V^{(3)}(\mathbf{P}_\alpha - \mathbf{P}_\beta)$$

$$[\delta_T(E_\alpha - E_\beta)]^2 = \frac{T}{2\pi} \delta_T(E_\alpha - E_\beta) \tag{2.23}$$

Also, in using the square of S-matrix elements as transition probabilities, we must take the states to be suitably normalized. In coordinate space, this means that instead of giving a one-particle state $|\Phi_\mathbf{p}\rangle$ of momentum $\mathbf{p}$ the wave function with continuum normalization

$$\langle \Phi_\mathbf{x} | \Phi_\mathbf{p} \rangle = \frac{e^{i\mathbf{p}\cdot\mathbf{x}}}{(2\pi)^{3/2}}$$

[17] we take it to be normalized so that the integral of its absolute-value squared *over the box* is unity:

$$\langle \Phi_\mathbf{x} | \Phi_\mathbf{p}^{\text{Box}} \rangle = \frac{e^{i\mathbf{p}\cdot\mathbf{x}}}{\sqrt{V}} \tag{2.24}$$

That is, we redefine the box-normalized state as

$$|\Phi_\mathbf{p}^{\text{Box}}\rangle \equiv \sqrt{\frac{(2\pi)^3}{V}} \, |\Phi_\mathbf{p}\rangle \tag{2.25}$$

For multiparticle states a product of factors of $\sqrt{(2\pi)^3/V}$ appears in the relation between box-normalized and continuum-normalized states. Hence, the S-matrix elements between box-normalized states are

$$S_{\beta\alpha}^{\text{Box}} = \left[\frac{(2\pi)^3}{V}\right]^{(N_\alpha + N_\beta)/2} S_{\beta\alpha} \tag{2.26}$$

---

[17]Here we use different convention because we assume the integral over momentum should be divided by $(2\pi)^3$ previously.

where N_α and N_β are the numbers of particles in the initial and final states, respectively. Putting this together, we see that the probability of the transition $\alpha \to \beta$ is

$$P(\alpha \to \beta) = \left| S_{\beta\alpha}^{\text{Box}} \right|^2$$

$$= \frac{T}{2\pi} \left[\frac{(2\pi)^3}{V} \right]^{N_\alpha + N_\beta - 1} \delta_V^{(3)}(\mathbf{P}_\alpha - \mathbf{P}_\beta) \delta_T(E_\alpha - E_\beta) \left| M_{\beta\alpha} \right|^2 \tag{2.27}$$

The transition *rate* is the transition probability divided by the time T during which the interaction is acting, or

2.3   The General Optical Theorem

Part II
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