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SCATTERING THEORY

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DESCRIPTION OF SCATTERING EVENTS

The fundamental structure and interactions of matter are investigated primarily by scattering experiments. Scattering theory provides the framework for systematic analysis of such experiments. Several references are available which provide detailed descriptions of scattering theory.[1,2,3,4]

A scattering experiment typically studies the collision of two kinds of particles[5], say P_1 and P_2, with respective initial momenta $\mathbf{p}_1$, and $\mathbf{p}_2$. We shall refer to P_1 as "beam particles" and P_2 as "target particles." In the "laboratory frame of reference" $\mathbf{p}_2 = 0$. Scattering events are classified on the basis of the final states observed after the collision has occurred.

In <u>elastic scattering</u> particles P_1 and P_2 are merely deflected, being observed to have final momenta $\mathbf{q}_1$ and $\mathbf{q}_2$ (indicated as $P_1 + P_2 \rightarrow P_1 + P_2$; an example is $e + H \rightarrow e + H$).

In <u>inelastic scattering</u> at least one of the particles is excited to an internal state which differs from that prior to the scattering (indicated as $P_1 + P_2 \rightarrow P_1^* + P_2$, etc.; an example is $e + H \rightarrow e + H^*$).

In a scattering reaction new particles emerge from the collision (indicated as $P_1 + P_2 \rightarrow Q_1 + Q_2$, $P_1 + P_2 \rightarrow Q_1 + \ldots + Q_N$; examples are $H + H \rightarrow p + e + H$ and $p + p \rightarrow p + n + \pi^+$). Since a given collision, involving P_1 and P_2 as the initial particles, can in general result in several alternate kinds of final states, it has been convenient to introduce the notion of "reaction channels" to classify the final state following the scattering. A particular channel is specified by the set of particles $Q_1, \ldots Q_N$ in the state.

The results of observations of scattering events are usually presented as scattering cross sections (when spin polarization is observed, other quantities are needed). To describe the scattering cross section, we suppose that a uniform flux F_B of beam particles P_1 (F_B represents the number of particles per unit area) has bombarded a "thin target" of particles P_2 ($\underset{\sim}{p}_2 = 0$). In the course of the experiment ΔN_{sc} scattering events have been detected. The scattering cross section $\Delta\sigma$ is defined then as

$$\Delta \sigma \;=\; \Delta N_{sc}/F_B. \qquad (1)$$

The detectors used in the experiment will ordinarily detect only certain specified kinds of particles and certain ranges of momenta for these, which accounts for the "Δ" in $\Delta \sigma$. If we sum over all ranges of final momenta and all possible kinds of final particles, (channels) we obtain from (1) the total cross section

$$\sigma = \sum_{\text{momenta}} \; \sum_{\text{channels}} \Delta \sigma. \qquad (2)$$

The number of events ΔN_{sc} is evidently a Lorentz invariant, being the same number to all observers. The beam flux F_B is also unchanged if we transform to another Lorentz frame moving parallel to $\underset{\sim}{p}_1$. The center of mass, or barycentric, frame of reference is that in which $\underset{\sim}{p}_1 = -\underset{\sim}{p}_2 \equiv \underset{\sim}{k}$. Evidently, $\Delta\sigma$ is the same in both the laboratory ($\underset{\sim}{p}_2 = 0$) and the barycentric frames of reference.[6]

There are some useful general properties of $\Delta\sigma$, which we now describe. First, the total energy E and the total momentum $\underset{\sim}{P}$ must be conserved in a collision. Thus, $\Delta\sigma$ must contain a factor

$$\delta(\underset{\sim}{P}_f - \underset{\sim}{P}_i)\, \delta(E_f - E_i)\,, \qquad (3)$$

where we have represented "initial" and "final" by the respective subscripts "i" and "f". We have noted that the detectors of final state particles will ordinarily record events for a restricted domain only of the momenta $\underset{\sim}{q}_1 \cdots \underset{\sim}{q}_N$. We therefore expect $\Delta\sigma$ to involve an integration,

$$\int d^3q_1 \ldots d^3q_N \ldots$$

over this domain set by the detectors. Since (1) and (3) are Lorentz invariants, and so is the ratio $d^3q_1/\varepsilon_{1q_1}$ (here $\varepsilon_{1q_1} = (M_1^2c^2 + q_1^2)^{\frac{1}{2}}c$, where ε_{1q_1} and M_1 are the energy and rest mass of Q_1). We can therefore write $\Delta\sigma$ in an evident invariant form as

$$\Delta\sigma \int \frac{d^3q_1}{\varepsilon_{1q_1}} \;\ldots\; \frac{d^3q_N}{\varepsilon_{Nq_N}} \;\delta(\underset{\sim}{P}_f - \underset{\sim}{P}_i)\, \delta(E_f - E_i)\; I. \qquad (4)$$

The quantity I above is an invariant function of $\mathbf{p}_1 \ldots \mathbf{q}_N$. It is dependent on the detailed dynanmics of the collision.

For elastic scattering in the center-of-mass frame we have $\mathbf{p}_1 = \mathbf{k} = -\mathbf{p}_2$, $\mathbf{q}_1 = \mathbf{k}' = -\mathbf{q}_2$, $k' = k$, and $\mathbf{k}\cdot\mathbf{k}' = k^2\cos\theta$. The invariant quantity I may then be taken as a function of the two variables k and θ, or $I = I(k,\theta)$. Alternatively, we can express I as a function of the two Mandelstam[7] variables

$$\begin{aligned} s &= (p_1 + p_2)^2 = (q_1 + q_2)^2 \\ t &= (p_1 - q_1)^2 = (p_2 - q_2)^2. \end{aligned} \tag{5}$$

[Here we have written the four-vector $(\mathbf{p}_1, \varepsilon_{1p_1})$ simply as p_1, etc.]

For elastic scattering in the barycentric frame (4) has the form

$$\Delta\sigma = \int \frac{d^3q_1\, d^3q_2}{\varepsilon_{1q_1}\,\varepsilon_{2q_2}}\, \delta(\mathbf{q}_1 + \mathbf{q}_2)\, \delta(\varepsilon_{1q_1} + \varepsilon_{2q_2} - \varepsilon_{1k} - \varepsilon_{2k})\, I$$

$$= \int \frac{d\,\Omega_1 q_1^2 d\,q_1}{\varepsilon_{1q_1}\,\varepsilon_{2q_2}}\, \delta(\varepsilon_{1q_1} + \varepsilon_{2q_1} - \varepsilon_{1k} - \varepsilon_{2k})\, I.$$

If the observed solid angle is sufficiently small that I can be evaluated at a single angle θ, we can remove $d\,\Omega_1$ from the integral and evaluate the q_1-integral to give the differential center-of-mass cross section as

$$\left(\frac{d\sigma}{d\,\Omega_1}\right)_{cm} = \left[(k/c^2)/(\varepsilon_{1k} + \varepsilon_{2k})\right] I\,(k,\theta). \tag{6}$$

The corresponding differential cross section in the laboratory frame may also be easily evaluated from (4). The laboratory frame moves parallel to $\mathbf{k}$ with a velocity

$$c\beta = c^2k/\varepsilon_{2k}, \quad \text{or} \quad \gamma = (1-\beta^2)^{-\frac{1}{2}} = \varepsilon_{2k}/(M_2c^2). \tag{7}$$

The total energies (kinetic plus rest energy) in the two frames are related by the useful expression

$$E_{cm}^2 = c^2\left[c^2(M_1^2 - M_2^2) + 2\,M_2\,E_{lab}\right]. \tag{8}$$

In the laboratory frame (4) is

$$\Delta\sigma = \int \frac{d^3q_1\, d^3q_2}{\varepsilon_{1q_1}\,\varepsilon_{2q_2}}\, \delta(\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{p}_1)\, \delta(\varepsilon_{1q_1} + \varepsilon_{2q_2} - \varepsilon_{1p_1} - M_2c^2) \times I.$$

Integration over $\mathbf{q}_2$ gives the result that $\mathbf{q}_2 = \mathbf{p}_1 - \mathbf{q}_1$. Division by the solid angle $d\,\Omega_1$ of particle P_1 and integration over q_2 gives us the differential cross section in the laboratory frame as

$$\left(\frac{d\sigma}{d\,\Omega_1}\right)_L = \frac{(q_1/c^2)\, I(k,\theta)}{\varepsilon_{1q_1}\,\varepsilon_{2|\mathbf{p}_1-\mathbf{q}_1|}} \left[\frac{q_1}{\varepsilon_{1q_1}} - \frac{\mathbf{q}_1\cdot(\mathbf{p}_1-\mathbf{q}_1)}{q_1\varepsilon_{2|\mathbf{p}_1-\mathbf{q}_1|}}\right]^{-1}. \tag{9}$$

Here $\varepsilon_{1q_1} + \varepsilon_{2|\mathbf{p}_1-\mathbf{q}_1|} = \varepsilon_{1p_1}$.

Since $I(k,\theta)$ is the same quantity in Eqs. (6) and (9), it may be eliminated to give the transformation equation between the differential cross sections in the laboratory and barycentric frames.

The kinematics of more general reactions may be discussed in a similar manner using Eq. (4).[8]

POTENTIAL SCATTERING

Nonrelativistic elastic scattering by a local, central potential $V(r)$ provides the simplest example of a collision of two particles. In the barycentric coordinate system the wavefunction $\psi_{\underset{\sim}{K}}^{+}$ may be expressed as a function of the relative particle coordinate $\underset{\sim}{r}$. The Schrödinger equation describing this interaction is[9]

$$\left[\nabla_r^2 + K^2 - v(r)\right] \psi_{\underset{\sim}{K}}^{+}(\underset{\sim}{r}) = 0. \quad (10)$$

Here $v(r) = 2M_r V(r)/\hbar^2$, with M_r the reduced mass of P_1 and P_2, and $\hbar \underset{\sim}{K}$ is the momentum of P_1 prior to the collision. Although scattering can be studied under more general conditions, the properties of (10) are simplified when

$$\int_0^\infty dr\, r|v(r)| < \infty,$$

$$\int_0^\infty dr\, r^2|v(r)| < \infty .$$

The continuum wavefunctions $\psi_{\underset{\sim}{K}}^{+}$ are conventionally normalized so that

$$(\psi_{\underset{\sim}{K}}^{+},\psi_{\underset{\sim}{P}}^{+}) = \delta(\underset{\sim}{K} - \underset{\sim}{P}) . \quad (12)$$

The $\psi_{\underset{\sim}{K}}^{+}$ and the bound state wavefunctions (if any) form a complete set of states in the reduced space from which the center-of-mass coordinates have been eliminated. The full two-body wavefunctions are of the form

$$\psi = (2\pi h)^{-\frac{3}{2}} \exp(i\underset{\sim}{P} \cdot \underset{\sim}{R})\, \psi_{\underset{\sim}{K}}^{+}(\underset{\sim}{r}), \quad (13)$$

where $\underset{\sim}{P}$ is the total momentum and $\underset{\sim}{R}$ is the center-of-mass coordinate of P_1 and P_2.

The asymptotic form of $\psi_{\underset{\sim}{K}}^{+}$, as Kr becomes very large, is

$$\psi_{\underset{\sim}{K}}^{+} \to (2\pi h)^{-\frac{3}{2}} \left[e^{i\underset{\sim}{K}\cdot\underset{\sim}{r}} + \left(e^{iKr}/r\right) f(\hat{\underset{\sim}{K}} \cdot \hat{\underset{\sim}{r}})\right]. \quad (14)$$

Here $f(\hat{\underset{\sim}{K}} \cdot \hat{\underset{\sim}{r}})$ is the <u>scattering amplitude</u> and describes the deflection of P_1 from the direction $\hat{\underset{\sim}{K}}$ to the direction $\hat{\underset{\sim}{r}}$. The barycentric scattering cross section (6) in this case has the explicit form

$$\left(\frac{d\sigma}{d\,\Omega_1}\right)_{cm} = |f(\hat{\underset{\sim}{K}} \cdot \hat{\underset{\sim}{r}})|^2. \quad (15)$$

The quantity I in (6) may be expressed in terms of $|f|^2$ using (15) and the cross section in the laboratory frame obtained using (9).

The partial wave expansion of $\psi_{\underset{\sim}{K}}^{+}$ is of the form

$$\psi_{\underset{\sim}{K}}^{+}(\underset{\sim}{r}) = \sum_{\ell=0}^{\infty} \left[(2\ell + 1)/(4\pi Kr)\right] i^{\ell} \exp\left[i\delta_\ell(K)\right]$$

$$\times\ P_\ell(\hat{\underset{\sim}{K}} \cdot \hat{\underset{\sim}{r}})\, w_\ell(K;r). \quad (16)$$

Here P_ℓ is the Legendre polynomial of order ℓ and $\delta_\ell(K)$ is the scattering phase shift. The radial wavefunction w_ℓ satisfies the ordinary differential equation

$$\left[\frac{d^2}{dr^2} + K^2 - \ell(\ell+1)/r^2 - v(r)\right] w_\ell = 0 \tag{17}$$

and is regular at the origin[10]. For Kr large w_ℓ has the asymptotic form

$$w_\ell(K;r) = (2/\pi)^{\frac{1}{2}} \sin(Kr - \pi\ell/2 + \delta_\ell(K)) . \tag{18}$$

The quantity

$$S_\ell(K) = \exp\left[2 i \delta_\ell(K)\right] \tag{19}$$

is an eigenvalue of Heisenberg's S-matrix.[11]

Another class of useful solutions of Eq. (15) are the Jost functions $f_\ell(\pm K;r)$. These satisfy the boundary conditions that as $Kr \to \infty$,

$$f_\ell(\pm K;r) \to i^\ell e^{\mp iKr} . \tag{20}$$

When the conditions (11) are satisfied the function $f_\ell(K;r)$ is analytic in K for $\mathrm{Im}(K) < 0$. Study of the Jost function has given insight into many general properties of collision processes and has stimulated extensions to relativistic quantum theory.[12]

SCATTERING BY NON-CENTRAL FORCES

We now suppose that P_1 and P_2 have respective spins S_1 and S_2, with z-components ν_1 and ν_2, and that the forces responsible for scattering also act on the spin orientation. If we write $u(\nu_1,\nu_2)$ for the spin wavefunction of P_1 and P_2, the asymptotic wavefunction (12) is modified to read

$$\psi^+_{\underset{\sim}{K}\,\nu_1\nu_2} \to (2\pi h)^{-\frac{3}{2}} \left[e^{i\underset{\sim}{K}\cdot\underset{\sim}{r}}\, u(\nu_1,\nu_2) + (e^{iKr}/r) \left\langle \nu_1',\nu_2' \middle| \underset{\sim}{f}(\hat{\underset{\sim}{K}} \cdot \hat{\underset{\sim}{r}}) \middle| \nu_1,\nu_2 \right\rangle u(\nu_1',\nu_2') \right. . \tag{21}$$

The scattering amplitude $\underset{\sim}{f}$ is now a $(2S_1 + 1)$ $(2S_2 + 1)$ square matrix. The cross section in the barycentric frame, with initial spin orientation (ν_1,ν_2) and final spin orientation (ν_1',ν_2'), is

$$\left(\frac{d\sigma}{d\,\Omega_1}\right)_{cm} = \left| \left\langle \nu_1',\nu_2' \middle| \underset{\sim}{f}(\hat{\underset{\sim}{K}} \cdot \hat{\underset{\sim}{r}}) \middle| \nu_1,\nu_2 \right\rangle \right|^2 . \tag{22}$$

For a scattering experiment in which ν_1' and ν_2' are not observed (22) should be summed over the $(2S_1 + 1) \times (2S_2 + 1)$ values of ν_1' and ν_2'. For an experiment with an unpolarized beam (22) should be averaged over ν_1 and ν_2.

When P_1 and/or P_2 are polarized prior to collision, it is often convenient to introduce a density matrix $\underset{\sim}{\rho}_i$ for the initial state:

$$\underset{\sim}{\rho}_i = \overline{u(\nu_1,\nu_2)\, u^\dagger(\nu_1,\nu_2)} , \tag{23}$$

where the bar indicates a suitably weighted average over ν_1 and ν_2. Evidently $T_r(\underset{\sim}{\rho}_i) = 1$. For unpolarized beam and target particles,

$\underset{\sim}{\rho}_i$ is just the identity matrix divided by $(2S_1 + 1) \times (2S_2 + 1)$.

The final state density matrix is

$$\underset{\sim}{\rho}_f = \underset{\sim}{f}\,\underset{\sim}{\rho}_i\underset{\sim}{f}^{\dagger}. \tag{24}$$

The scattering cross section, summed over all final spin orientations, is

$$\left(\frac{d\sigma}{d\,\Omega_1}\right)_{cm} = \mathrm{Tr}\,(\underset{\sim}{\rho}_f). \tag{25}$$

The average value of the spin vector $\underset{\sim}{S}_1$, for example, is

$$\overline{\underset{\sim}{S}}_1 = \mathrm{Tr}(\underset{\sim}{S}_1\underset{\sim}{\rho}_f/\mathrm{Tr}(\underset{\sim}{\rho}_f). \tag{26}$$

Following two sequential scatterings, the density matrix is

$$\underset{\sim}{\rho}_f = \underset{\sim}{f}_2\underset{\sim}{f}_1\underset{\sim}{\rho}_i\underset{\sim}{f}_1^{\dagger}\underset{\sim}{f}_2^{\dagger}. \tag{27}$$

Here $\underset{\sim}{f}_1$ is the scattering amplitude for the first and $\underset{\sim}{f}_2$ that for the second scattering.[13]

FORMAL SCATTERING THEORY

A powerful, formal description applicable to relativistic and many particle collisions, has developed following work of Heisenberg,[14] Moller,[15] Lippmann and Schwinger,[16] Gell Mann and Goldberger,[17] and many others. To describe scattering from an initial state χ_i to a final state χ_f a scattering matrix $\mathfrak{T}_{fi}$ is introduced. If V is the quantity in the Hamiltonian responsible for the scattering and ψ_i^+ is the time-independent wavefunction describing the complete event, then

$$\mathfrak{T}_{fi} = (\chi_f, V\,\psi_i^{+}). \tag{28}$$

Taking account of momentum conservation we can write this as

$$\mathfrak{T}_{fi} = \delta(\underset{\sim}{P}_f - \underset{\sim}{P}_i)\, T_{fi}\,, \tag{29}$$

where T_{fi} is a scattering matrix defined only in the subspace for which total momentum is conserved.

The cross section (4) can be expressed in terms of the reduced scattering matrix T_{fi} with the identification (here v_{net} is the relative velocity of the two particles P_1 and P_2 in the initial state "i")

$$I = \left[\frac{(2\pi)^4\hbar^2}{v_{rel}}\right] |T_{fi}|^2\,(\varepsilon_{iq_1}\,\ldots\,\varepsilon_{Nq_N}). \tag{30}$$

Heisenberg's[14] unitary <u>S-matrix</u> is related to $\mathfrak{T}_{fi}$ by the relation[18]

$$S_{fi} = \delta_{fi} - 2\pi\, i\, \delta(E_f - E_i)\,\mathfrak{T}_{fi}. \tag{31}$$

With a suitable scaling factor (associated with the normalization of the states χ_i and χ_f) S is invariant under Lorentz transformations. It is, as mentioned, unitary and is in general consistent with certain symmetries and conservation laws (for example, total angular momentum and total charge). The extent to which S is determined by such general considerations, independently of the Schrödinger equation, has been given extensive study.[19]

SCATTERING FROM COMPLEX PARTICLES

Scattering of two particles, when one or both are complex systems (such as atoms or molecules) involves a multi-particle interaction. Collisions involving complex particles may be elastic (in which case P_1 and P_2 may formally be treated as if simple, non-complex particles), inelastic, or lead to reactions in which different particles Q_1, Q_2 ... Q_N appear. Exact, analytic solutions cannot be given when three or more particles interact. Thus, the scattering of complex systems must be treated by approximate and/or numerical methods.

When the kinetic energy of the colliding particles is high compared with their internal binding energies, the impulse approximation [20,21] is often useful. In this approximation the scattering of a simple particle by a complex particle is treated as if the complex particle consisted of an assemblage of non-interacting free particles and the T-matrix is replaced by a sum of two-particle T-matrices. The scattering is averaged over the momentum spectra of the initial state χ_i. The sum over final states depends on the process being considered, but often may be evaluated in the closure approximation.[22]

The optical model[23] provides a technique which is frequently convenient for describing elastic scattering from complex particles. In this model the actual many-body interaction is replaced by an equivalent two-body interaction (in principle this is exact if the correct equivalent interaction were known) in the Schrödinger equation.

An elegant technique for studying three-particle interactions (for example, e + H or n + D scattering) has been proposed

by Fadeev.[24,25] Numerical techniques have been applied to Fadeev's equations with some success.[26]

A very extensive literature exists relating to the scattering of electrons, protons, ions, and atoms by atoms or molecules.[27,28] Relative good approximations (usually relying on numerical computation) are available for studying scattering of electrons by the lighter atoms.[4,25,26] Semi-classical techniques may be applicable for studying slow collisions of protons and ions with light atoms.[29,30] The more complex phenomena which occur when heavy atoms or molecules scatter, or when the complex structure of both P_1 and P_2 must be taken into account are often studied by heuristic methods, crude approximations, and/or experiments.

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9. The notation here is that of Ref. (3).
10. For a more complete discussion see, for example, Eq. (6.120) of Ref. (3).
11. See, for example, Chap. 7 of Ref. (2) for a thorough discussion of the S-matrix.
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