2

Diffraction Theory

There are two principal assumptions that underlie Fraunhofer diffraction theory. The first of these is that the wavelength of the incident field be much smaller than the size of any aperture through which it passes. In the three-dimensional scattering problems that interest us, this becomes the condition that the wavelength be smaller than the range of any of the forces that deflect the incident particle. A second condition is less familiar in the optical context, where refractive effects are often negligible or even absent, but it is equally important for more general sorts of scattering processes. It is that the kinetic energy of the incident particle be sufficiently high that the force fields that it encounters tend to lead mainly to small deflections.

Under these conditions nearly all of the scattered intensity is projected into a diffraction pattern close to the forward direction. If $\boldsymbol{k}$ and $\boldsymbol{k}'$ are the initial and final propagation vectors of the projectile wave function, or alternatively the initial and final momenta divided by $\hbar$, the momentum transfers $\hbar\boldsymbol{q} = \hbar(\boldsymbol{k}' - \boldsymbol{k})$ will tend characteristically to be small in magnitude, $q/k \ll 1$. The distribution of these momentum transfers may nonetheless be quite informative about the force fields responsible for the scattering processes.

As long as our two assumptions hold true, incident particles will tend to pass through the region of interaction with little deflection, that is to say they will continue, at least approximately, to follow straight-line paths through the interaction region. Let us assume that the incident projectile is described by the plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ and that the nuclear force can be described for the present by a static potential of some sort. Then in the region lying in the "shadow" of the potential, i.e., for points lying beyond the potential, but not too far from it, the wave function can be approximated as $\exp[i\boldsymbol{k}\cdot\boldsymbol{r} + i\chi(\boldsymbol{b})]$, where $\boldsymbol{b}$ is an impact vector, the component of $\boldsymbol{r}$ perpendicular to $\boldsymbol{k}$, and χ is a phase shift function that describes the cumulative effect of passage through the potential.

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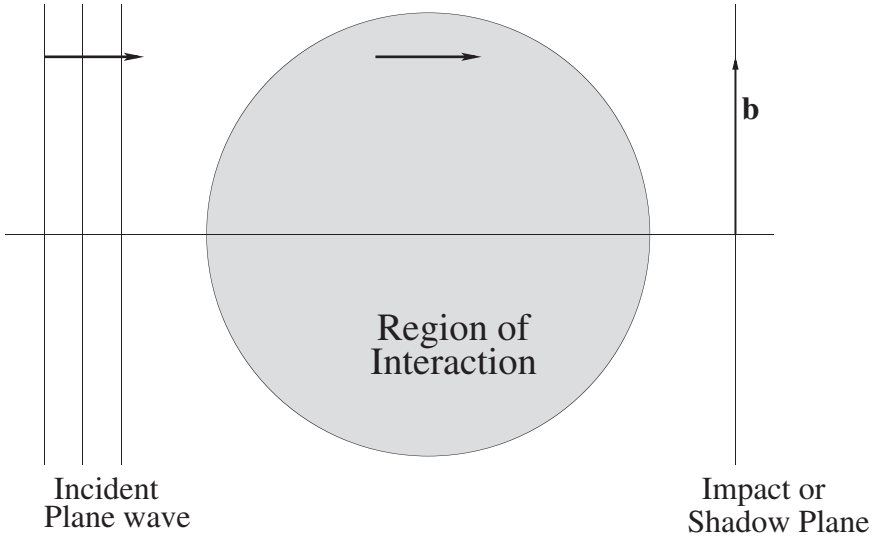


Figure 2.1 Geometry of the scattering process.

It is convenient to imagine constructing a shadow or impact plane perpendicular to $\boldsymbol{k}$ in the region immediately shadowed by the nuclear interaction, i.e., close to the nucleus but just beyond its range of interaction, so that the lateral spreading of the wave function components may remain quite small. (See Fig. 2.1.) If we take the wave function in that plane to be $\exp[i\boldsymbol{k}\cdot\boldsymbol{r}+i\chi(\boldsymbol{b})]$ and then apply Green's theorem to evaluate the wave function in the half-space beyond it, we can find the scattering amplitude from the form it takes far from the plane. For small momentum transfers, that scattering amplitude is given by [8]

$$f(\boldsymbol{k}',\boldsymbol{k}) = \frac{ik}{2\pi}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{b}}\left\{1-e^{i\chi(\boldsymbol{b})}\right\}\mathrm{d}^2b. \tag{2.1}$$

The integration over impact vectors $\boldsymbol{b}$ in this expression can be thought of as being carried out over the impact plane. The scattering amplitude Eq. (2.1) is in fact a slightly generalized form of the familiar Kirchhoff integral for the amplitude of Fraunhofer diffraction. It possesses a number of derivations other than the one we have outlined [8], and each of these seems to suggest other generalizations, or to have mathematical advantages of its own. We shall confine ourselves here simply to mentioning several of them.

When the function $\chi(\boldsymbol{b})$ has azimuthal symmetry, for example, about the direction $\boldsymbol{k}$, i.e., when $\chi = \chi(b)$ the angular integral in Eq. (2.1) may be expressed in terms of the Bessel function J_0. We then have [1]

$$f(\boldsymbol{k}',\boldsymbol{k}) = ik\int_0^\infty J_0(qb)\left\{1-e^{i\chi(b)}\right\}b\,\mathrm{d}b, \tag{2.2}$$

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an integral that may be regarded as the high-energy limit of the general expression for a scattering amplitude as a sum of spherical harmonic functions [12,16,20]. We have included a brief discussion of this expansion and its relation to the diffraction theory in Appendix A. We need only note here that the impact parameter b corresponds to the angular momentum ℓ (for ℓ sufficiently large) through $kb = \ell + \frac{1}{2}$.

The representation of nuclear forces by a simple static potential would, if taken literally, be a considerable oversimplification. An incident high energy particle has an appreciable chance, as a rule, of exciting the nucleus and leaving some part of its energy behind. Such processes bring about a decrease in amplitude of the part of the wave function propagating at the incident energy and it is from that part that we calculate the elastic scattering amplitude. Inelastic scattering, in other words, is a loss mechanism and its effect can be represented by letting the phase shift function $\chi(b)$ have a positive imaginary part. (That representation amounts, in the simplest optical diffraction experiments, to letting $\exp\{i\chi(\boldsymbol{b})\}$ be zero wherever an absorbing screen obstructs the wave, and letting it equal unity within any open aperture.)

It would go far beyond our present needs to delve into the theory of nuclear forces, but a further element of generality present in Eq. (2.1) is surely worth mentioning. The representation of the nuclear interaction by means of a complex phase shift function $\chi(\boldsymbol{b})$ is considerably more general than its description by means of a potential $V(\boldsymbol{r})$, be it real or complex. Not all field interactions can be described accurately by means of a local potential, but under the assumptions we have stated there must be a phase shift function $\chi(\boldsymbol{b})$, whether there exists such a local potential or not.

If the interaction is indeed describable by means of a local scalar potential $V(\boldsymbol{r})$ then, within the context of the Klein–Gordon equation, the phase shift function is given approximately by [8]

$$\chi(\boldsymbol{b}) = -\frac{1}{\hbar v}\int_{-\infty}^{\infty} V(\boldsymbol{b} + \hat{\boldsymbol{\kappa}} z)\,\mathrm{d}z \tag{2.3}$$

where $\hat{\boldsymbol{\kappa}}$ is the unit vector $\hat{\boldsymbol{\kappa}} = \boldsymbol{k}/k$ and v is the velocity of the incident particle. If V is a spherically symmetric potential, $V = V(r)$, this expression reduces to

$$\chi(b) = -\frac{1}{\hbar v}\int_{-\infty}^{\infty} V\left(\sqrt{b^2 + z^2}\right)\mathrm{d}z \tag{2.4}$$

$$= -\frac{2}{\hbar v}\int_{b}^{\infty} \frac{V(r) r\,\mathrm{d}r}{\sqrt{r^2 - b^2}} \tag{2.5}$$

If the analysis of experimental data were somehow to furnish us with an azimuthally symmetric phase shift function $\chi(b)$ we could then regard Eq. (2.5) as an integral equation to determine a corresponding local and spherically symmetric

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potential $V(r)$. The integral equation, Eq. (2.5), is in fact of the Abel variety and possesses the explicit solution [8]

$$V(r) = \frac{\hbar v}{\pi r}\frac{\mathrm{d}}{\mathrm{d}r}\int_r^\infty \frac{\chi(b) b\,\mathrm{d}b}{\sqrt{b^2 - r^2}} \tag{2.6a}$$

$$= \frac{\hbar v}{\pi}\frac{\mathrm{d}}{\mathrm{d}(r^2)}\int_{-\infty}^{\infty} \chi\left(\sqrt{r^2 + z^2}\right)\mathrm{d}z \tag{2.6b}$$

$$= \frac{\hbar v}{2\pi}\int_{-\infty}^{\infty} \frac{\chi'\left(\sqrt{r^2 + z^2}\right)}{\sqrt{r^2 + z^2}}\,\mathrm{d}z. \tag{2.6c}$$

This is, in effect, an "optical potential," equivalent to the phase shift function $\chi(b)$ in the sense that it leads to the same scattering amplitude. It is often unclear, however, whether the "optical potential" has any physical meaning deeper than that. In the present approach, therefore, we shall give considerably greater emphasis to the phase shift function $\chi(\boldsymbol{b})$ which stands, after all, in a much closer relation to experimental observation.

A further point concerning the approximate scattering amplitude, Eq. (2.1), is worth noting. A number of analyses have shown that the angular range of the approximation can be extended somewhat [22] by taking the vector $\hat{\boldsymbol{\kappa}}$ to be in the direction of the vector $\frac{1}{2}(\boldsymbol{k} + \boldsymbol{k}')$, rather than $\boldsymbol{k}$, and by taking the impact plane to be perpendicular to it. We have illustrated this choice in Fig. 2.2, which shows $\hat{\boldsymbol{\kappa}} = (\boldsymbol{k} + \boldsymbol{k}')/|\boldsymbol{k} + \boldsymbol{k}'|$ and the two auxiliary vectors, $\hat{\boldsymbol{q}} = (\boldsymbol{k}' - \boldsymbol{k})/|\boldsymbol{k}' - \boldsymbol{k}|$ and

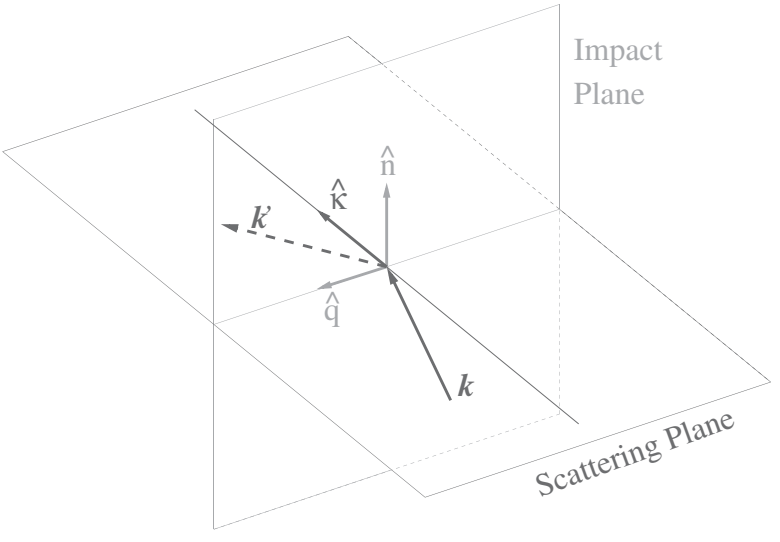


Figure 2.2 Coordinate system used.

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$\hat{\boldsymbol{n}} = \boldsymbol{k} \times \boldsymbol{k}'/|\boldsymbol{k} \times \boldsymbol{k}'|$. These are mutually orthogonal unit vectors. They have been defined to form a right-handed triad in the sense that $\hat{\boldsymbol{q}} \times \hat{\boldsymbol{n}} = \hat{\boldsymbol{\kappa}}$.[1]

Scattering amplitudes such as that of Eq. (2.1) possess several symmetry properties that will be useful to us at later points. They are invariant under velocity reversal,

$$f(-\boldsymbol{k}, -\boldsymbol{k}') = f(\boldsymbol{k}', \boldsymbol{k}), \tag{2.7}$$

a relation that is equivalent to "time reversal" symmetry, an invariance under reversal of both the order and the signs of the initial and final momenta. It holds only when the phase shift function $\chi(\boldsymbol{b})$ is real-valued. Furthermore, for interactions that are also invariant under coordinate inversion we have $\chi(-\boldsymbol{b}) = \chi(\boldsymbol{b})$ and consequently

$$f(-\boldsymbol{k}, -\boldsymbol{k}') = f(\boldsymbol{k}, \boldsymbol{k}') \tag{2.8}$$

so that the scattering amplitude according to Eq. (2.7) then has the symmetry

$$f(\boldsymbol{k}', \boldsymbol{k}) = f(\boldsymbol{k}, \boldsymbol{k}'). \tag{2.9}$$

The scattering amplitude, Eq. (2.1), also possesses an interesting symmetry that is quite specific to the diffraction approximation from which it stems. If we write the amplitude $f(\boldsymbol{k}', \boldsymbol{k})$ as a function of the phase shift function χ and the vector $\boldsymbol{q}$, i.e.,

$$f(\boldsymbol{k}', \boldsymbol{k}) = \mathcal{F}[\chi, \boldsymbol{q}],$$

then the transformation $\boldsymbol{q} \to -\boldsymbol{q}$ and $\chi \to -\chi^*$ (which preserves the absorptive character of the phase shift function) carries the scattering amplitude into its complex conjugate and changes its sign,

$$\mathcal{F}[-\chi^*, -\boldsymbol{q}] = -\mathcal{F}^*[\chi, \boldsymbol{q}]. \tag{2.10}$$

In particular then, if the phase shift function is symmetric under spatial inversion, and furthermore purely imaginary, the scattering amplitude obeys the relations

$$\mathcal{F}[\chi, -\boldsymbol{q}] = \mathcal{F}[\chi, \boldsymbol{q}] = -\mathcal{F}^*[\chi, \boldsymbol{q}], \tag{2.11}$$

which show it must then be purely imaginary.

[1] The sign of $\boldsymbol{q}$ is opposite to that used in [3].

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