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Asymptotic Diffraction Theory and Classical Scattering

It is quite instructive, as a first step in exploring the asymptotic behavior of the differential scattering amplitude, to observe the way in which it approaches its classical limit for real-valued interactions. We can simplify the expression in Eq. (2.1) a bit for that purpose by noting that it contains the two-dimensional delta function[1]

$$\frac{1}{2\pi}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{b}}\,\mathrm{d}^2b = 2\pi\,\delta^{(2)}(\boldsymbol{q}), \tag{3.1}$$

which is known when defined with suitable care to vanish for $\boldsymbol{q} \neq 0$. To evaluate the integral Eq. (2.1) for the scattering amplitude, in other words, we will need only to fix our attention on the remaining term, the two-dimensional Fourier transform of $\exp\{i\chi(\boldsymbol{b})\}$, and to take the same care in carrying out the required integration. Neither the expression Eq. (3.1) for the delta function, nor the Fourier transform of $\exp\{i\chi(\boldsymbol{b})\}$ is a properly convergent integral, however, until we proceed a bit more cautiously by defining them, for example, by means of an appropriate summation convention.

For interactions of finite range, for example, we do not change the scattering amplitude $f(\boldsymbol{k}',\boldsymbol{k})$ of Eq. (2.1) by defining it as the limit

$$f(\boldsymbol{k}',\boldsymbol{k}) = \lim_{\epsilon\to 0}\frac{ik}{2\pi}\int e^{-\epsilon b^2 - i\boldsymbol{q}\cdot\boldsymbol{b}}\left\{1 - e^{i\chi(\boldsymbol{b})}\right\}\mathrm{d}^2\boldsymbol{b}, \tag{3.2}$$

taken as ϵ goes to zero through positive values. While this limiting procedure does not change the scattering amplitude, it does give a unique definition for arbitrarily

[1] The Dirac delta function [6] $\int \mathrm{d}x \exp(-iqx) = 2\pi\,\delta(q)$ is defined as vanishing save in the neighborhood of $q = 0$, and yet providing the integral $\int \mathrm{d}q\,\delta(q) = 1$. We have used the symbol $\delta^{(2)}(\boldsymbol{q})$ for the two-dimensional version of the function defined on the $\boldsymbol{q}$-plane.

small ϵ to the two terms that make it up. In particular, the delta function in Eq. (3.1) is replaced by

$$\frac{1}{2\pi}\int e^{-\epsilon b^2 - i\boldsymbol{q}\cdot\boldsymbol{b}}\,\mathrm{d}^2\boldsymbol{b} = \frac{1}{2\epsilon}e^{-\frac{q^2}{4\epsilon}}, \tag{3.3}$$

which becomes vanishingly small for $q \gg 2\sqrt{\epsilon}$. The scattering amplitude for $q \gg 2\sqrt{\epsilon}$ is then given by the well-defined integral

$$f(\boldsymbol{k}',\boldsymbol{k}) = \lim_{\epsilon\to 0}\frac{k}{2\pi i}\int \exp\{-\epsilon b^2 - i\boldsymbol{q}\cdot\boldsymbol{b} + i\chi(\boldsymbol{b})\}\,\mathrm{d}^2\boldsymbol{b}. \tag{3.4}$$

In the classical limit, $\hbar \to 0$, the de Broglie wavelength of the incident particle goes to zero. The magnitude of the vector $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$ for any fixed angle of scattering then becomes infinite. The phase shift $\chi(b)$, as we can see from Eq. (2.3), also becomes infinite in magnitude, and may be expected to vary rapidly with the position $\boldsymbol{b}$ as well. The principal contributions to the integral in Eq. (3.4) are bound therefore to come from the immediate neighborhoods of the points at which the phase $-\boldsymbol{q}\cdot\boldsymbol{b} + \chi(\boldsymbol{b})$ is stationary. These are the points in the impact plane which satisfy the relation

$$\nabla_b\{-\boldsymbol{q}\cdot\boldsymbol{b} + \chi(\boldsymbol{b})\} = 0$$

or

$$\boldsymbol{q} = \nabla_b\chi(\boldsymbol{b}). \tag{3.5}$$

The classical significance of this stationary phase condition is immediately clear. If a particle at the position $\boldsymbol{r} = \boldsymbol{b} + \hat{\boldsymbol{\kappa}}z$ is subject to a potential $V(\boldsymbol{b} + \hat{\boldsymbol{\kappa}}z)$ then it experiences a transverse force $-\nabla_b V(\boldsymbol{b} + \hat{\boldsymbol{\kappa}}z)$. The integral of this force over time, according to Eq. (2.3), is given by $\hbar\nabla_b\chi(\boldsymbol{b})$. That transverse impulse then must represent the transfer of momentum to the scattered particle,

$$\hbar(\boldsymbol{k}' - \boldsymbol{k}) = \hbar\boldsymbol{q} = \hbar\nabla_b\chi(\boldsymbol{b}). \tag{3.6}$$

This is precisely the stationary phase condition in Eq. (3.5). It possesses only a discrete set of roots for the impact vector $\boldsymbol{b}$. There is, in other words, at most only a discrete set of classical trajectories, if indeed there are any at all, that can lead to scattering for any given momentum transfer $\hbar\boldsymbol{q}$.

To find the roots of Eq. (3.5) it is convenient to adopt a coordinate system within the impact plane. We can use the unit vectors $\hat{\boldsymbol{q}}$ and $\hat{\boldsymbol{n}}$ defined in connection with Fig. 2.2 to write

$$\boldsymbol{b} = \hat{\boldsymbol{q}}b_x + \hat{\boldsymbol{n}}b_y, \tag{3.7}$$

and express the phase shift as a function of its Cartesian coordinates, $\chi(b_x, b_y)$. The stationary points are then determined by the pair of equations

$$\frac{\partial}{\partial b_x}\chi(b_x, b_y) = q \tag{3.8}$$

$$\frac{\partial}{\partial b_y}\chi(b_x, b_y) = 0. \tag{3.9}$$

The phase shift functions we encounter most often are rotationally invariant,

$$\chi(\boldsymbol{b}) = \chi(b) = \chi\left(\sqrt{b_x^2 + b_y^2}\right), \tag{3.10}$$

and in that case Eqs. (3.8) and (3.9) reduce to

$$\frac{b_x}{b}\chi'(b) = q \tag{3.11a}$$

$$\frac{b_y}{b}\chi'(b) = 0. \tag{3.11b}$$

The latter of these equations shows that either b_y or $\chi'(b)$ must be zero. If $\chi'(b)$ were to vanish, however, there could be no stationary point for finite q according to Eq. (3.11a). A stationary point for $q \neq 0$, therefore, can only occur for $b_y = 0$, i.e., for $\boldsymbol{b}$ lying in the scattering plane. The coordinate b_x is then determined by what remains of Eq. (3.11),

$$\frac{b_x}{|b_x|}\chi'(|b_x|) = q. \tag{3.12}$$

Of course, when the phase shift function lacks this rotational symmetry, the stationary points could lie anywhere in the impact plane.

We can approximate the scattering amplitude, Eq. (3.4), by expanding the phase shift function in its integrand in the neighborhood of its stationary points. If $\boldsymbol{b}_0$ is a stationary point, for example, we can write, in dyadic notation (i.e., double scalar product)

$$\chi(\boldsymbol{b}) - \boldsymbol{q}\cdot\boldsymbol{b} = \chi(\boldsymbol{b}_0) - \boldsymbol{q}\cdot\boldsymbol{b}_0 + \tfrac{1}{2}(\boldsymbol{b}-\boldsymbol{b}_0)(\boldsymbol{b}-\boldsymbol{b}_0) : \nabla_b\nabla_b\chi(\boldsymbol{b})\Big|_{\boldsymbol{b}_0}. \tag{3.13}$$

For the special case of rotational symmetry $\chi(\boldsymbol{b}) = \chi(b)$ we have

$$\nabla_b\nabla_b\chi(\boldsymbol{b}) = \frac{\boldsymbol{b}}{b}\frac{\boldsymbol{b}}{b}\chi''(b) - \frac{\boldsymbol{b}\boldsymbol{b}}{b^3}\chi'(b) + \frac{\mathbb{I}}{b}\chi'(b), \tag{3.14}$$

where $\mathbb{I}$ stands for the unit dyadic, $\hat{\boldsymbol{q}}\hat{\boldsymbol{q}} + \hat{\boldsymbol{n}}\hat{\boldsymbol{n}}$. It is convenient to introduce Cartesian coordinates centered at the stationary point $\boldsymbol{b}_0$ by writing

$$\boldsymbol{b} - \boldsymbol{b}_0 = \hat{\boldsymbol{q}}x + \hat{\boldsymbol{n}}y \tag{3.15}$$

so that we have

$$\tfrac{1}{2}(\boldsymbol{b}-\boldsymbol{b}_0)(\boldsymbol{b}-\boldsymbol{b}_0):\nabla_b\nabla_b\chi(\boldsymbol{b})\Big|_{\boldsymbol{b}_0}=\alpha_x x^2+\alpha_y y^2, \tag{3.16}$$

and the phase function can be written as

$$\chi(\boldsymbol{b})-\boldsymbol{q}\cdot\boldsymbol{b}=\chi(\boldsymbol{b}_0)-\boldsymbol{q}\cdot\boldsymbol{b}_0+\alpha_x x^2+\alpha_y y^2, \tag{3.17}$$

where

$$\alpha_x \equiv \tfrac{1}{2}\chi''(|b_{0x}|) \tag{3.18a}$$

$$\alpha_y = \chi'(|b_{0x}|)/2|b_{0x}| = q/2b_{0x}. \tag{3.18b}$$

The contribution of the stationary point $\boldsymbol{b}_0$ to the scattering amplitude, Eq. (3.4), can now be written as

$$f_0(\boldsymbol{k}',\boldsymbol{k})=\frac{k}{2\pi i}\,e^{-i\boldsymbol{q}\cdot\boldsymbol{b}_0+i\chi(b_0)}\,\mathcal{I}_0(\boldsymbol{q}), \tag{3.19}$$

where

$$\mathcal{I}_0(\boldsymbol{q})=\lim_{\epsilon\to 0}\int e^{-\epsilon(x^2+y^2)+i\alpha_x x^2+i\alpha_y y^2}\,\mathrm{d}x\,\mathrm{d}y \tag{3.20}$$

is a Gaussian integral to be carried out over the impact plane. Its two Cartesian factors are given by

$$\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} e^{-(\epsilon-i\alpha_y)y^2}\,\mathrm{d}y=\left(\frac{i\pi}{\alpha_y}\right)^{\frac{1}{2}} \tag{3.21a}$$

and

$$\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} e^{-(\epsilon-i\alpha_x)x^2}\,\mathrm{d}x=\left(\frac{i\pi}{\alpha_x}\right)^{\frac{1}{2}}. \tag{3.21b}$$

The integral $\mathcal{I}_0(\boldsymbol{q})$ is therefore given by the product

$$\begin{aligned}\mathcal{I}_0(\boldsymbol{q})&=\frac{\pi}{(-\alpha_x\alpha_y)^{\frac{1}{2}}}\\&=2\pi\left(\frac{-b_{0x}}{\chi'(b_{0x})\chi''(b_{0x})}\right)^{\frac{1}{2}}.\end{aligned} \tag{3.22}$$

The contribution of the assumed stationary point $\boldsymbol{b}_0$ to the scattering amplitude, Eq. (3.4), can thus be written as

$$f_0(\boldsymbol{k}',\boldsymbol{k})=\frac{k}{i}\left(\frac{-b_{0x}}{q\chi''(b_{0x})}\right)^{\frac{1}{2}} e^{-iqb_{0x}+i\chi(b_{0x})} \tag{3.23}$$

where we have made use of Eq. (3.11) to substitute q/b_{0x} for $\chi'(b_{0x})/b_{0x}$. To avoid ambiguities of sign for the actual physical scattering amplitude we must be careful to specify which branch of the square root factor is to be used in this expression. We take it to be the branch for which $\{e^{i\theta}\}^{\frac{1}{2}} = e^{\frac{1}{2}i\theta}$ for $-\pi < \theta \le \pi$. The scattering amplitude must retain the diffraction symmetry we have stated in Eq. (2.10) and that furnishes an important check on the consistency of the phases in Eq. (3.23).

If we do not assume rotational symmetry it is necessary to integrate the exponential function of a more general quadratic form, but that can easily be done and yields the more general result

$$f_0(\boldsymbol{k}', \boldsymbol{k}) = \frac{k}{\left\{\det \nabla_b \nabla_b \chi(\boldsymbol{b})\big|_{\boldsymbol{b}_0}\right\}^{\frac{1}{2}}} \exp\{i[-\boldsymbol{q} \cdot \boldsymbol{b}_0 + \chi(\boldsymbol{b}_0)]\}. \tag{3.24}$$

The determinant in this expression is that of the matrix of second derivatives of the phase shift function $\chi(\boldsymbol{b})$ evaluated at the stationary point $\boldsymbol{b}_0$.

It is quite interesting to compare this quantum-mechanical result with the classical cross section. To find the classical cross section we need only know the element of solid angle into which the incident particle is projected when it impinges on the element of area $\mathrm{d}\sigma = \mathrm{d}^2\boldsymbol{b}$ of the impact plane in the neighborhood of $\boldsymbol{b}$. The momentum transfer $\hbar q$ and the impact vector $\boldsymbol{b}$ are related by the classical Eq. (3.6) (which is also the stationary phase condition). It follows then that an element of area $\mathrm{d}^2\boldsymbol{b}$ is related to a two-dimensional element of $\boldsymbol{q}$-vectors via

$$\mathrm{d}^2\boldsymbol{b} = \frac{\partial(\boldsymbol{b})}{\partial(\boldsymbol{q})}\, \mathrm{d}^2\boldsymbol{q} \tag{3.25}$$

in which $\partial(\boldsymbol{b})/\partial(\boldsymbol{q})$ is a Jacobian determinant,

$$\frac{\partial(\boldsymbol{b})}{\partial(\boldsymbol{q})} = \frac{1}{\left|\det \nabla_b \nabla_b \chi(\boldsymbol{b})\right|_{\boldsymbol{b}_0}} \tag{3.26}$$

evaluated at the point $\boldsymbol{b}_0$. Since the element of solid angle $\mathrm{d}\Omega$ is given near the forward direction by $\mathrm{d}^2\boldsymbol{q} = k^2\,\mathrm{d}\Omega$, we find that the classical differential cross section is

$$\frac{\mathrm{d}\sigma_0}{\mathrm{d}\Omega} = k^2 \frac{\partial(\boldsymbol{b})}{\partial(\boldsymbol{q})}\bigg|_{\boldsymbol{b}_0} \tag{3.27a}$$

$$= \frac{k^2}{|\det \nabla_b \nabla_b \chi(\boldsymbol{b})|_{\boldsymbol{b}_0}}. \tag{3.27b}$$

This is, of course, precisely the squared absolute value of the quantum mechanical scattering amplitude Eq. (3.24).

We have assumed in the example just considered that there is only one point of stationary phase on the entire $\boldsymbol{b}$-plane. This means, in the classical limit, that only one particle trajectory corresponds to any value of the momentum transfer $\boldsymbol{q}$ and it is then no surprise that the differential cross section, when evaluated quantum mechanically, agrees closely with the classical result. When there are more trajectories that correspond classically to any value of $\boldsymbol{q}$, the quantum mechanical scattering amplitude will be a sum of terms f_j that introduce interference effects into the scattered intensity

$$f(\boldsymbol{k}',\boldsymbol{k}) = \sum_j f_j(\boldsymbol{k}',\boldsymbol{k}). \tag{3.28}$$

We shall show presently that these additional trajectories are supplied by further points of stationary phase in the plane of impact vectors $\boldsymbol{b}$, and that they are responsible for the presence of additional terms in the scattering amplitude, Eq. (3.28).

For the larger momentum transfers to which the asymptotic approximation applies most accurately it can provide dramatic insights into the behavior of scattering cross sections. It will frequently happen, for example, that Eq. (3.5) for the stationary phase point, or the equivalent Eq. (3.6) for the classical theory, possesses no solution for some range of momentum transfer vectors $\boldsymbol{q}$. In that case it is often possible to continue the phase function $\chi(\boldsymbol{b})$ analytically into a space of complex $\boldsymbol{b}$-vectors, to find stationary points in that space and then to carry out the necessary integrations by complex extensions of the same method we have illustrated. When applied in that way the method will furnish the quantum mechanical amplitudes for scattering processes that have lowered probabilities because they are classically forbidden.

It is also important, as we have noted in the Introduction, to be able to deal with intrinsically complex phase shift functions $\chi(\boldsymbol{b})$. Such phase shift functions also lead us inevitably to discuss complex values for the impact vectors $\boldsymbol{b}$. Indeed, they furnish a natural description of the absorptive effects brought about by inelastic scattering.

Our asymptotic technique for evaluating the scattering amplitude is not without limitations, however, and one is already evident in the calculations we have done. We have had to assume that the magnitude of $\boldsymbol{q}$ is large in order to justify using the method of stationary phase, and that limitation means we must not evaluate the scattering amplitude too close to the forward direction. The value of developing the asymptotic approximation further in order to correct it near the forward direction is indeed somewhat questionable since that is where it is easiest to evaluate the integral, Eq. (2.1), by more elementary and traditional means. It is also where the integral tends to present the least information about the spatial dependence of the interaction.

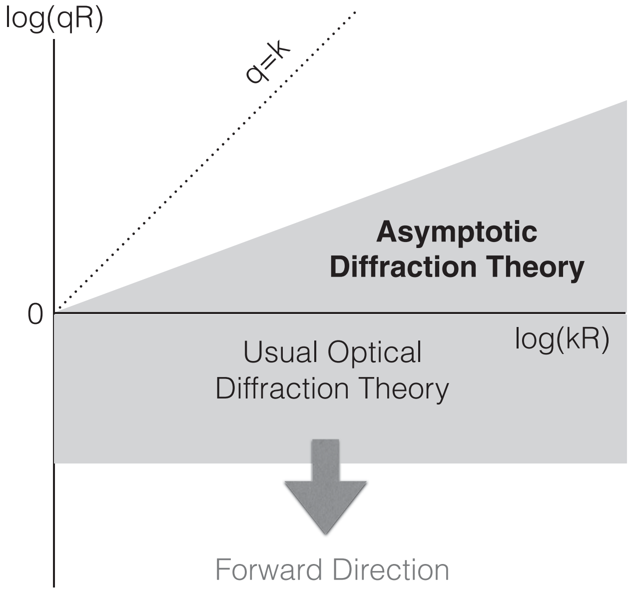

Figure 3.1 The region where the usual optical diffraction theory applies extends down to $\log(qR) \to -\infty$. The wedge $qR > 1$ contains the domain where the asymptotic theory is applicable. The size of the scattering target is represented by R, whereas the beam momentum and momentum transfer are denoted k and q, respectively.

To summarize in more mathematical terms, diffraction theory rests upon the two assumptions

$$q \ll k, \quad 1 \ll kR, \tag{3.29}$$

where R is a characteristic size of the scattering target, whereas the asymptotic limit also requires q to be large, $1 \ll qR$, or

$$\frac{1}{R} \ll q \ll k. \tag{3.30}$$

This regime, shown as a triangle in Fig. 3.1, is where our asymptotic considerations will apply.