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1981 J. Phys. A: Math. Gen. 14 165

(http://iopscience.iop.org/0305-4470/14/1/016)

J. Phys. A: Math. Gen. **14** (1981) 165–171. Printed in Great Britain

Electron diffraction by a cylindrical capacitor

W L Schaich†

Institut für Festkörperforschung, Kernforschungsanlage Jülich, Postfach 1913, D-5170 Jülich, West Germany‡

Received 24 January 1980, in final form 28 May 1980

Abstract. The diffraction of electrons by a cylindrical capacitor is formulated in terms of conventional quantum scattering theory. Using several approximations valid in the short wavelength limit, the theory is reduced to a form that allows direct comparison with formulae based on the diffraction integral, thereby clarifying the content of the latter. A recent, alternative treatment of the same problem is shown to be in error.

1. Introduction

The diffraction of electrons around macroscopic objects provides clear evidence for the wave-like nature of matter (Komrska 1971). A particular example of such well established experiments is the interference pattern produced by an electrostatic biprism. As first described by Möllenstedt and Düker (1955, 1956), a diverging electron beam is sent around a metallised filament placed between two grounded plates, thereby separating the beam into two parts. By applying a positive potential to the filament, the two parts of the beam are then made to recombine in the observation plane, where they produce an interference pattern whose detailed structure depends on the strength of the applied potential.

At the simplest level of analysis, one can understand the separation of extrema in the pattern by comparing the path length difference for classical trajectories that pass on one side or the other of the filament (Donati *et al* 1973). This approach is easy to apply and is readily extended to more complex situations, as for instance to include a magnetic field. Yet it is also of interest to develop a more detailed analysis that allows a quantitative treatment of the complete pattern for the simplest configuration. Such a treatment has been derived from the diffraction integral approach, which itself is adapted from optics; see Komrska (1971) for a review of this theory. Here one relates the electron wavefunction in the observation plane to reasonable estimates of its values in a plane perpendicular to the incident direction and passing through the filament axis. The comparison of this theory with experiment is quite impressive (Komrska 1971).

Still it is of theoretical interest to consider this model problem from other points of view. We present here a treatment derived from the conventional theory of quantum scattering by symmetric objects, which is based on phase shifts and an angular momentum sum. Our aim is not only to show that this approach can be carried through but also to use it to clarify several aspects of the diffraction integral theory. Work with a

† Work supported in part by NSF through grant No. DMR 78-10235.

‡ Permanent address: Physics Department, Indiana University, Bloomington, IN 47401, USA.

0305-4470/81/010165+07$01.50

similar goal was recently presented by Gesztesy and Pittner (1979), but unfortunately their results are flawed, as we shall discuss later.

In § 2, we present the derivation of our basic formulae and in § 3 we describe the calculation of the necessary phase shifts. Section 4 contains our discussion and conclusions.

2. Formal theory

The essential configuration of the scattering experiment is shown in figure 1. In this idealised picture the potential is cylindrically symmetric and independent of the third dimension, so we may treat the scattering process as two-dimensional. The incident beam is considered to emerge from a point source at I, pass through the region of finite potential, $a \leqslant |\boldsymbol{x}| = x \leqslant b$, which is centred on the origin of the filament, and be detected along the arc $\boldsymbol{x}_o$. Electrons that strike the filament, $x < a$, will be assumed to be removed from the beam, while those beyond $x = b$ feel no potential. We neglect the finite width of the source and detector as well as the small range of electron energies. Such effects may be incorporated by an appropriate average of our results (Drahos and Delong 1964).

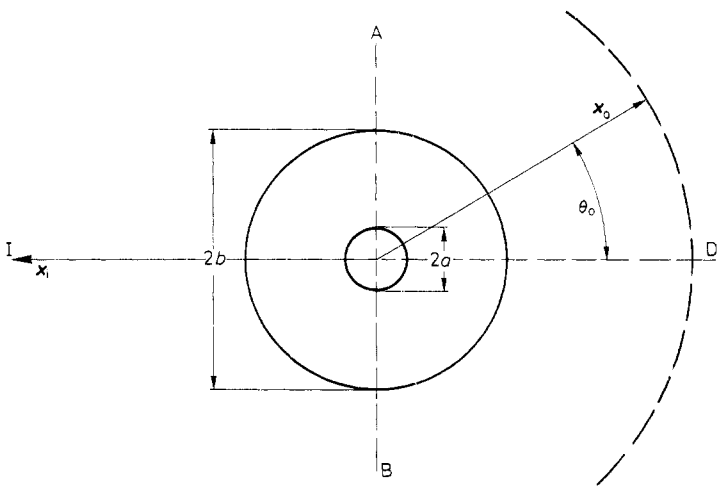

Figure 1. Sketch of idealised experimental configuration. The distance scales are distorted because in practice $x_i, x_o \gg b \gg a$. See text for further description.

The key assumptions for our analysis are that the potential energy, V, is cylindrically symmetric and of finite range, for they allow us a tractable decomposition of the wavefunction into angular momentum components. The scattered wave solution may be written as

$$\psi = (1 + G_o^+ T^+)\phi, \tag{2.1}$$

where ϕ is the incident wave, G_o^+ the outgoing free-particle Green function, and T^+ the t-matrix associated with V. To represent the diverging incident wave, we choose

$$\phi(\boldsymbol{x}) = H_o^{(1)}(k|\boldsymbol{x} - \boldsymbol{x}_i|), \tag{2.2}$$

where $k = (2mE)^{1/2}/h$ with E the energy and m the mass of the electron, and $H_o^{(1)}$ is a cylindrical outgoing wave (Abramowitz and Stegun 1964). Then expanding both G_o^+ and T^+ in terms of appropriate angular harmonics, $e^{il\theta}$, with θ measured from the axis ID (Morse and Feshbach 1953), we obtain, when x_i and x_o are greater than b, the range of the potential,

$$\psi(\boldsymbol{x}_o) = H_o^{(1)}(k|\boldsymbol{x}_o - \boldsymbol{x}_i|) + \sum_{l=-\infty}^{\infty} e^{il\theta_o} H_l^{(1)}(kx_o) \tfrac{1}{2}(e^{2i\delta_l} - 1) H_l^{(1)}(kx_i)\, e^{-il\theta_i}, \tag{2.3}$$

where $H_l^{(1)}$ are Bessel functions (Abramowitz and Stegun 1964), $\theta_i = \pi$ and δ_l is the phase shift for the lth partial wave. It is defined by the requirement that the l-wave solution of Schrödinger's equation which is regular at the origin becomes a constant times $e^{i\delta_l} H_l^{(1)}(kx) + e^{-i\delta_l} H_l^{(2)}(kx)$ for x beyond the range of V.

The approach leading to (2.3) is formally exact and is merely the two-dimensional analogue of well known three-dimensional theory (Lloyd and Smith 1972). The difficulty in its exact solution here is that the sum on l extends to values of the order of kb, which can be as large as 10^9 (Komrska 1971). We hence apply the following approximate scheme which was developed for the scattering of neutral atoms by macroscopic cylinders (Mehl and Schaich 1980). First rewrite the second term in (2.3) as the difference of two expressions:

$$F\{\delta_l\} = \tfrac{1}{2} \sum_{l=-\infty}^{\infty} H_l^{(1)}(kx_o) H_l^{(1)}(kx_i)\, e^{2i\delta_l}\, e^{il(\theta_o - \pi)} \tag{2.4}$$

and

$$F_o = F\{\delta_l \equiv 0\}. \tag{2.5}$$

Although both F and F_o are divergent sums, due to the lack of the cut-off provided by $(e^{2i\delta_l} - 1)$ at large $|l|$, these infinities will cancel in forming $F - F_o$. Our interest lies with the finite contribution to them coming from $|l|/k$ smaller than x_o or x_i. For F_o, which is independent of the potential energy V, one may confidently proceed with a semiclassical attack: replace the l sum by an integral and evaluate the finite part of the integral by the stationary phase approximation. Using the asymptotic expansions (Abramowitz and Stegun 1964)

$$H_l^{(1)}(z) = \frac{(2/\pi)^{1/2}}{(z^2 - l^2)^{1/4}} \exp\left[i\left((z^2 - l^2)^{1/2} + l \sin^{-1}\frac{l}{z} - \frac{\pi}{2} l - \frac{\pi}{4} \right) \right] (1 + O(z^2 - l^2)^{-1/2}), \tag{2.6}$$

we find a stationary phase point in the F_o expression at

$$l_p = -kx_o x_i \sin\theta_o / |\boldsymbol{x}_o - \boldsymbol{x}_i| \tag{2.7}$$

about which we expand the phase to second order in $l - l_p = \Delta l$. An integral over all Δl then yields

$$F_o \approx H_o^{(1)}(k|\boldsymbol{x}_o - \boldsymbol{x}_i|), \tag{2.8}$$

i.e. the finite part of F_o that is not identically cancelled by F reproduces the incident wave. For (2.8) to be valid both kx_o and kx_i must be large and $|l_p|$ must be much smaller than either of them. From (2.7) we see that this latter condition only holds in the forward direction, but in typical experiments θ_o is never more than 10^{-3} rad (Komrska 1971), so it is easily satisfied here. The utility of (2.8) is that it implies that the total wavefunction is well approximated by the finite part of $F\{\delta_l\}$.

The evaluation of F by the same means as used for F_o is in general not as easily justified. One must examine the variation of the phase shift with l. We postpone this until the next section and here simply write F as an integral over l. Further, we make several simplifying approximations: we expand the l dependence of the Bessel functions (2.6) to low order and set the scattered intensity proportional to $k|\psi(x_o)|^2$ (Komrska 1971), to find

$$I/I_o \approx \left| \int_{-\infty}^{\infty} dl \exp[i(l\theta_o + l^2/2kr + 2\delta_l)] \right|^2 / 2\pi kr \tag{2.9}$$

where $1/r = 1/x_o + 1/x_i$ and I/I_o is the ratio of the flux at x_o with and without the capacitor being present. This formula, like (2.8), is only valid in the forward direction and there should be no large $|l|$ contributions (i.e. from $|l| \sim kr$) because of rapid phase oscillations. In this way, we separate off the finite physical contribution to F.

Equation (2.9) allows a preliminary comparison with the diffraction integral result for this model problem (Komrska 1971, equation (161)). There the analogue of the integral over l is expressed as an integral over $-k\xi$, where ξ is an effective impact parameter measured from the filament centre in the diffraction plane, i.e. along the line AB in figure 1. For a detailed comparison of the two formulae we need to find the δ_l.

3. Phase shifts

In the same spirit as the derivation of § 2, we shall estimate the phase shifts using WKB theory. There is a qualitative change in the phase shift when $|l|$ passes through ka. For $|l|$ smaller than ka, an electron in its radial motion encounters no turning points until it strikes the surface, where we assume it is lost from the beam. This means that an incoming cylindrical wave produces essentially no outgoing cylindrical wave, so

$$\exp(2i\delta_l^{WKB}) \approx 0, \qquad |l| \leqslant ka. \tag{3.1}$$

On the other hand for $|l| > ka$, there is an outermost turning point, r_t, which, as $|l|$ increases, moves well above the surface. Applying the simple WKB connection formulae (Newton 1966) at this turning point, we obtain

$$|\exp(2i\delta_l^{WKB})| \approx 1 \tag{3.2}$$

and specifically

$$\delta_l^{WKB} = \int_{r_t}^{\infty} q(r)\, dr - \int_{|l|/k}^{\infty} q_o(r)\, dr, \qquad |l| > ka, \tag{3.3}$$

where

$$q(r) = k[1 - l^2/k^2r^2 - V(r)/E]^{1/2}, \qquad q(r_t) = 0, \tag{3.4}$$

$$q_o(r) = k[1 - l^2/k^2r^2]^{1/2}, \qquad q_o(|l|/k) = 0. \tag{3.5}$$

Thus the WKB phase shift is just the shift in phase calculated with and without V. We have written approximate equalities in (3.1) and (3.2) because the change in behaviour is actually spread out over a range of l. There exist more sophisticated WKB theories (Berry and Mount 1972, Fröman and Fröman 1965) that allow one to describe this transition, but for their evaluations we would need to know the detailed form of V near

$r = a$. Here we simply use

$$V(r) = \epsilon \ln r/b, \qquad \epsilon = |e|\phi/\ln a/b, \tag{3.6}$$

where $|e|\phi$ is the potential energy difference between a and b, since a rough estimate using in addition an image potential in V shows that the transition region is only about $\Delta l/k \sim 1$ Å wide, whereas $a \sim 10^3$ Å (Komrska 1971). We also neglect the shift in the location of the transition region with the applied potential, since experimentally $\epsilon/E \ll 1$.

From our results one sees that $|e^{2i\delta_l}|$ is the analogue of the transmission function used in the diffraction integral approach (Komrska 1971). An advantage of the present formalism is that one can systematically improve its calculation, although for this particular problem it is well approximated by a step function. We also remark that Gesztesy and Pittner (1979) used a different boundary condition in their analysis: perfect reflection rather than complete absorption on the filament surface.

To evaluate (3.3) we use the identity (Newton 1966)

$$\mathrm{d}\delta_l^{\mathrm{WKB}}/\mathrm{d}l = -\tfrac{1}{2}\Phi(l), \tag{3.7}$$

where $\Phi(l)$ is the classical deflection angle for an electron of angular momentum lh. We roughly estimate Φ by calculating the transverse momentum given to an electron moving along its unperturbed trajectory (Landau and Lifshitz 1960). Then integrating (3.7) and using (3.6) we obtain

$$2\delta_l^{\mathrm{WKB}} \approx -\frac{\epsilon}{E}\frac{k}{2}\int_0^{(b^2-\xi^2)^{1/2}} \mathrm{d}x \ln\left(\frac{\xi^2+x^2}{b^2}\right), \qquad kb > |l| = k|\xi| > ka,$$

$$= \frac{\epsilon}{E} kb[(1-\xi^2 b^2)^{1/2} - \xi/b \cos^{-1} \xi/b]. \tag{3.8}$$

Since the important values of $|l|$ in (2.9) are much less than kb, we expand (3.8) to

$$2\delta_l^{\mathrm{WKB}} \approx \frac{\epsilon}{E}\left[kb - |l|\left(\frac{\pi}{2} - \frac{|l|}{2kb} - \frac{|l|^3}{24k^3b^3} + \ldots\right)\right]. \tag{3.9}$$

A simpler way to the limiting result is to note that the deflection angle is for $ka < |l| \ll kb$ essentially independent of l (Donati *et al* 1973):

$$|\Phi_l| \sim \tfrac{1}{2}\pi\epsilon/E \ll 1, \tag{3.10}$$

so by (3.7)

$$2\delta_l^{\mathrm{WKB}} \sim \text{constant} - \tfrac{1}{2}|l|\pi\epsilon/E, \qquad ka < |l| \ll kb. \tag{3.11}$$

We stress that the various approximations that lead from (3.3) to (3.11) are not required by our method, but instead are appropriate to the model problem we consider here. In the atom scattering problem one had to resort to a full solution of Schrödinger's equation to obtain sufficiently accurate values of δ_l (Mehl and Schaich 1980).

If we substitute (3.9) and (3.1) into (2.9), we obtain to within a phase factor Komrska's diffraction integral result (Komrska 1971, equation (16i)). The discrepancy in phase is given by

$$-\frac{\epsilon}{2E}|l|\left(\frac{|l|}{kr} - \theta_0\right)\ln\left(\frac{|l|}{kb}\right). \tag{3.12}$$

It results in our language from Komrska's use of an alternate trajectory for calculating

Φ, and hence δ. His approach is similar in spirit to the two-asymptote approximation for Φ discussed by Fulcher *et al* (1976), but since (3.12) involves r and θ_0 it cannot be obtained as a correction to δ_l, which depends only on the scattering potential. In any case (3.12) makes merely a small change in the l variation of the phase in (2.9), and the experiment is not sufficiently accurate to demonstrate its presence.

We conclude this section by noting that even for $|l| > ka$ the phase-shift formulae of Gesztesy and Pittner (1979) do not agree with ours. For the analogue of (3.11), they find (see their equation (4.6)) a faster than exponential fall-off with $|l|$ and no dependence on ϵ/E. Their method involves approximating a polynomial series representation of the exact solution of Schrödinger's equation, and it is not clear from their brief description where an error arises. We can only say that the approximate wavefunction they present in their (3.6) leads directly to their (4.6), which disagrees with our (3.11). This error leads them in subsequent analysis of the scattered intensity to predictions that disagree with previous theory and experiment (Komrska 1971). For instance, their (8.10) claims that the motion of the Fresnel pattern is quadratic, rather than linear, in the applied potential.

4. Discussion

Coupling the phase shifts of § 3 with equation (2.9), one can now evaluate the scattered intensity. Note that the variation with l of (3.8) is sufficiently weak to justify using the integral in (2.9). Further, if one uses the limiting form (3.11), the required integrals are of the Fresnel type (Abramowitz and Stegun 1964). However, we do not present such calculations here but instead refer the reader to Komrska's evaluation of the diffraction integral (Komrska 1971), which as we have shown is essentially equivalent to (2.9). We only remark that the primary features of the interference pattern can be understood by a stationary phase evaluation of (2.9).

To summarise, for the particular model problem of the electrostatic biprism, our derivation reproduces the diffraction integral results. We have presented the derivation in the spirit of a semiclassical approximation with no quantitative estimate of the error. Such estimates can be made (Mehl 1980, unpublished), but they are numerically unimportant for the problem treated here. We feel that it is more important to focus on the prescriptions for what is to be calculated and to appreciate the different point of view offered by our approach.

It is remarkable that the sum of incident plus scattered waves in (2.3) combine to yield a single expression (2.4) for the total wavefunction. We have checked that such a cancellation of the incident wave in the forward direction also occurs for an incident plane wave, and for analogous situations in three dimensions with a spherically symmetric V.

For calculational purposes it is reassuring that the transmission factor and phase differences of the diffraction integral can be expressed in terms of the δ_l, for the accuracy of the latter can be systematically improved. There is no limitation of (2.9) to weak potential energies, except that one might have to sum over l rather than integrate. However, independent of potential strength, (2.9) only holds in the forward direction (specifically when $|l_p|$ of (2.7) is much less than kr) and is helpful only in the Fresnel limit $ka^2 \gg r$, which applies in the experiments considered here.

The fact that our approach, whose existence depends on the cylindrical shape of the scatterer, agrees with the diffraction integral, which neglects its shape, is heuristically

satisfying. Yet this is also the weakest point of our approach: it is limited to configurations of high symmetry. The diffraction integral has a much wider range of useful applications (Komrska 1971).

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