## **Appendix II**

# Light optics, electron optics and wave mechanics

In 1831 William Rowan Hamilton discovered the analogy between the trajectory of material particles in potential fields and the path of light rays in media with continuously variable refractive index. By virtue of its great mathematical beauty, the 'Hamiltonian Analogy' survived in the textbooks of dynamics for almost a hundred years, but did not inspire any practical applications until 1925 when H. Busch first explained the focusing effect of electric and magnetic fields on electron beams in optical terms. Almost at the same time E. Schrödinger took the Hamiltonian Analogy a step further by passing from geometrical optics to wave optics of particles with his wave equation, in which he incorporated the wavelength of particles, first conceived by Louis de Broglie in 1923.

Practical electron optics developed rapidly from 1928 onwards. By this time the Hamiltonian Analogy was widely known and inspired the invention of electron-optical counterparts of light-optical instruments, such as the electron microscope. Though the mathematical analogy is general, the two techniques are not exactly parallel. Some electron-optical instruments such as cathode-ray tubes and systems with curved optic axes have no important counterparts in light optics. In the available space only those problems of electron optics will be considered whose light-optical analogues were developed at length in the previous chapters of this work, so that the results can be transferred almost *in toto*, with few modifications. It may be noted that this applies in particular to the most recondite chapter of electron optics: the wave theory of lens aberrations.

#### 1 The Hamiltonian analogy in elementary form

We will show first that the determination of the trajectory of a charged particle can be reduced to an optical problem by the introduction of a suitable refractive index, variable from point to point.

Consider a particle of charge e and of mass m, to which we will for the sake of simplicity refer as an electron, moving in a steady electrostatic potential field  $\phi(x, y, z)$ . By Newton's law of motion

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = e\mathbf{E} = -e\,\mathrm{grad}\,\phi,\tag{1}$$

where **p** is the momentum vector. This law is valid at all velocities **v** if Newton's definition of the momentum  $\mathbf{p} = m\mathbf{v}$  is replaced by Einstein's

$$\mathbf{p} = \frac{m\mathbf{v}}{\sqrt{1 - \beta^2}}, \qquad \left(\beta = \frac{v}{c}\right),\tag{2}$$

c being the vacuum velocity of light.

It is convenient to split the equation of motion (1) into two equations, of which one is the equation of the trajectory, while the other specifies the 'time table' according to which the electron moves along the trajectory. For this purpose we write  $\mathbf{v} = v\mathbf{s}$ ,  $\mathbf{p} = p\mathbf{s}$ ,  $\mathbf{s}$  being the unit vector in the direction of motion. Then

$$\frac{d\mathbf{p}}{dt} = \frac{dp}{dt}\mathbf{s} + p\frac{d\mathbf{s}}{dt} = \frac{dp}{dt}\mathbf{s} + p\frac{d\mathbf{s}}{ds}\frac{ds}{dt} = \frac{dp}{dt}\mathbf{s} + pv\frac{d\mathbf{s}}{ds}.$$

Now it is well known from differential geometry that ds/ds is a vector in the direction of the unit principal normal v, whose absolute value is equal to the curvature  $1/\rho$  of the trajectory. Hence

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \frac{\mathrm{d}p}{\mathrm{d}t}\mathbf{s} + \frac{pv}{\rho}\mathbf{v}.$$

From this relation and from (1) it follows that the instantaneous centre of curvature is in the plane which passes through the tangent  $\mathbf{s}$  and the electric vector  $\mathbf{E} = -\operatorname{grad} \phi$ . Resolving grad  $\phi$  in the two directions it follows that

$$\frac{\mathrm{d}p}{\mathrm{d}t}\mathbf{s} + \frac{pv}{\rho}\mathbf{v} = -e[(\mathbf{s} \cdot \operatorname{grad}\phi)\mathbf{s} + (\mathbf{v} \cdot \operatorname{grad}\phi)\mathbf{v}]. \tag{3}$$

Equating the first terms on the two sides we obtain a scalar equation, which can be called the 'time table,' because ultimately it leads to the position of the electron on the trajectory as function of time. After multiplying it by v = ds/dt, it can be integrated and gives

$$\frac{mc^2}{\sqrt{1-\beta^2}} = -e\phi + \text{constant.} \tag{4}$$

This is Einstein's energy integral. For slow-moving particles ( $\beta \ll 1$ ), it goes over into Newton's integral,  $\frac{1}{2}mv^2 + e\phi = \text{constant}$ .

We now restrict the problem, for convenience, by considering only electrons with the same integration constant, i.e. with the same total energy. This is the case if all electrons have started at a certain potential surface  $\phi_0$  with zero velocity. In many practical problems this surface can be identified with the cathode. Writing

$$V = \phi - \phi_0$$

i.e. measuring the potential V from this level, the energy integral now appears in the form

$$mc^2\left(\frac{1}{\sqrt{1-\beta^2}}-1\right) = -eV. \tag{4a}$$

Combining this with (2) we can express both in the form of a useful double equation

$$\left(1 - \frac{eV}{mc^2}\right)^2 = 1 + \left(\frac{p}{mc}\right)^2 = \frac{1}{1 - \beta^2}.$$
 (5)

Thus the scalar value p of the momentum of these particles is determined as a function of the position x, y, z by

$$mc^{2}\left[\sqrt{1+\left(\frac{p}{mc}\right)^{2}}-1\right]=-eV(x, y, z). \tag{6}$$

Consider now the second part of (3), i.e. the component at right angles to the direction of motion:

$$\frac{pv}{\rho} = -e[\mathbf{v} \cdot \operatorname{grad} V]. \tag{7}$$

Expressing v and V in terms of p by means of (2) and (6) we obtain the simple law

$$\frac{1}{\rho} = \frac{\mathbf{v} \cdot \operatorname{grad} p}{p} = \mathbf{v} \cdot \operatorname{grad}(\ln p). \tag{8}$$

Eq. (8) is identical with  $\S 3.2$  (14) for the curvature of rays in a medium of refractive index n, that is proportional to p, and we thus obtain a formal analogy between the paths of electrons and of light.

It must be emphasized that the absolute value p of the momentum is a function of position alone only for electrons of a fixed total energy; for electrons of a different energy it is another function, given by (6). Thus the refractive index is dependent on the electron energy. This too has its analogue in light optics, in the dependence of the refractive index on the colour of light. It will be shown later that this is a very appropriate analogy, as in both cases the refractive index turns out to be a function of the wavelength.

For slow electrons p is proportional to the velocity, and this in turn is proportional to  $\sqrt{V}$ . The relativistic equations which we have used have the advantage that they clearly indicate that it is the momentum, and not the velocity, which is the characteristic quantity. Moreover, these results immediately suggest a generalization for the case of a general static field, electric and magnetic. It is well known in relativity theory that in the presence of a magnetic field one must replace the mechanical momentum  $\mathbf{p}$ , which now we will write  $\mathbf{p}_m$ , by the 'total' momentum

$$\mathbf{p}_{\text{tot}} = \mathbf{p}_m + e\mathbf{A},\tag{9}$$

where **A** is the vector potential.\* This suggests that the refractive index, which in the electrostatic case was the component of  $\mathbf{p}_m$  in the direction of the motion, will have to be replaced in the general case by the component of  $\mathbf{p}_{tot}$  in the same direction. This guess proves to be correct, but it will now be preferable to place electron optics in electromagnetic fields on a more solid and general foundation.

<sup>\*</sup> It is remarkable that this fundamental result was discovered by K. Schwarzschild (Königl. Gess. Wiss. Göttingen, Math. Phys. Kl., 3 (1903), 126), three years before the advent of relativity.

#### 2 The Hamiltonian analogy in variational form

The laws of geometrical optics may be derived from Fermat's principle ( $\S 3.3.2$ ), according to which the path of light between two points  $P_1$  and  $P_2$  makes the optical length a minimum,

$$\int_{P_1}^{P_2} n \, \mathrm{d}s = \min. \tag{10}$$

It may be recalled that this *strong* formulation of Fermat's principle is valid only if the two end points are sufficiently close together, that is to say if there is no image of either  $P_1$  or  $P_2$  between these points on the ray connecting them. If  $P_2$  is the image of  $P_1$ , (10) does not determine a ray but an infinitesimal pencil of rays connecting the two points, each with the same optical length. If  $P_1$  and  $P_2$  are drawn farther apart, so that an image appears between them, the *weak* formulation

$$\delta \int_{P_1}^{P_2} n \, \mathrm{d}s = 0 \tag{10a}$$

again determines a ray, but this represents not a maximum, as is sometimes erroneously stated, but a stationary value of the integral, which is neither a minimum, nor a maximum.

Some consequences of Fermat's principle were discussed in §11 of Appendix I, on the calculus of variations. In §12 of Appendix I it was shown that the motion of a system of material points can be described in a similar variational form, by Hamilton's principle, which for the special case of a single material point is expressed by the condition

$$\int_{P_{1},t_{1}}^{P_{2},t_{2}} L(\dot{x},\dot{y},\dot{z},x,y,z) dt = \min.$$
 (11)

This formulation is valid in any system of coordinates, but for illustration Cartesian coordinates, x, y, z, will suffice  $\dot{x}$ ,  $\dot{y}$ ,  $\dot{z}$  are the velocity components, L is the Lagrangian function. Departure and arrival are specified in four-dimensional space-time, and are assumed to be fixed in the variational process. It was shown in Appendix I how the equations of motion in the Lagrangian and in the Hamiltonian form can be deduced as consequences of the principle (11) [Appendix I, (77), (78)].

For a relativistic electron, with charge e and rest mass m, the Lagrangian function is

$$L = -mc^2 \sqrt{1 - \beta^2} - e \left( \phi - \frac{1}{c} \dot{\mathbf{r}} \cdot \mathbf{A} \right). \tag{12}$$

Here  $\dot{\mathbf{r}} = \mathbf{v}$  is the velocity vector,  $\phi$  is the electrostatic potential, and  $\mathbf{A}$  the magnetic or vector potential.\* The Lagrangian (12) can be verified by substituting it into the Lagrangian equations of motion [Appendix I (77)] and making use of the electromagnetic relations §2.1 (7) and §2.1 (5),

$$\mathbf{E} = -\frac{1}{c}\dot{\mathbf{A}} - \operatorname{grad}\phi, \qquad \mathbf{B} = \operatorname{curl}\mathbf{A}.$$

<sup>\*</sup> The Lagrangian (12) without the relativistic corrections was found by K. Schwarzschild, *loc. cit.*, in 1903.

The Lagrangian equations then appear in the form

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = e\left(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}\right),\tag{13}$$

which is the Newton-Lorentz form of the equations of motion.

Hamilton's principle expressed by (11) is too general for the purpose of electron optics. It contains the time, which is without interest if the fields are stationary. Moreover, it represents  $\infty^5$  extremals;  $\infty^4$  because at given total energy the points  $P_1$ ,  $P_2$  can be freely chosen on any two given surfaces, and a further infinity because the total energy has been left undetermined. In order to reduce the cumbersome dimensionality similar steps are taken in electron optics as in light optics.

First we fix the energy constant, that is to say we restrict the discussion to monochromatic light or monoenergetic electrons. As shown in Appendix I (87) this allows a reduction by one in the dimensionality of the problem. Hamilton's principle (11) is now replaced by the principle of least action,

$$J = \int_{P_{1}, t_{1}}^{P_{2}, t_{2}} (L + E) dt = \min,$$
 (14)

where E is the total energy

$$E = \sum \dot{x} p_x - L.$$

In (14) the time t appears only in a formal way, because on substituting for E one obtains

$$J = \int_{P_1, t_1}^{P_2, t_2} \sum p_x \, \dot{x} \, dt = \int_{P_1}^{P_2} \sum p_x \, dx = \int_{P_1}^{P_2} \mathbf{p} \cdot d\mathbf{r} = \min.$$
 (15)

In the second and third expression we have dropped  $t_1$ ,  $t_2$ , because we are dealing with time-invariant fields only (otherwise the total energy would not remain constant), and in such fields the starting time  $t_1$  is of no consequence, while the transit time  $t_2 - t_1$  is fully determined by the path and by the energy constant.

Thus the principle of least action (14) is a complete analogue of Fermat's principle (10). The study of electron motion is reduced to an optical problem, if one defines the *electron-optical refractive index* as the *component of the momentum in the direction of the trajectory*. For a purely electrostatic field this result is seen to be equivalent to that found from more elementary considerations in the previous section. In this case the momentum is purely mechanical, and parallel to the trajectory, its value being given by (2):

$$p_m = \frac{mv}{\sqrt{1-\beta^2}}.$$

In the presence of a magnetic field we must use the general definition of momentum components [Appendix I (74)], as derivatives of the Lagrangian with respect to the velocity components. For a single particle with the Lagrangian (12) these are

$$p_x = \frac{\partial L}{\partial \dot{x}} = \frac{m\dot{x}}{\sqrt{1 - \beta^2}} + \frac{e}{c}A_x,$$

etc. In vector form

$$\mathbf{p} = \frac{m\mathbf{v}}{\sqrt{1-\beta^2}} + \frac{e}{c}\mathbf{A}.\tag{16}$$

Thus, apart from an arbitrary constant factor, the general electron-optical refractive index is

$$n = \frac{mv}{\sqrt{1 - \beta^2}} + \frac{e}{c} \mathbf{A} \cdot \mathbf{s},\tag{17}$$

where  $\mathbf{A} \cdot \mathbf{s}$  is the component of the vector potential in the direction of motion. Again it is understood that this must be interpreted as a function of position for electrons of a given total energy.

There appears to exist an important difference between the general case and the special case of purely electric fields. In an electric field the refractive index is proportional to the mechanical momentum, which is a measurable physical quantity. In the general expression (17) the second term is a component of the vector potential, which is not a physical quantity but a function, such that its *curl* is equal to the magnetic induction **B**. This makes it clear that the general electron-optical refractive index itself is not a physical quantity, but a Lagrangian function.\* But this is equally true of the special refractive index in a purely electric field. In both cases we could add to it the component, in the direction of motion, of the gradient of any arbitrary function of position, without altering any of the physical consequences.

There exists a more important difference between the special and the general case, which is best explained if now we follow further the simplifying procedure of optics, and reduce the  $\infty^4$  manifoldness of trajectory fields to  $\infty^2$ . We do this by selecting those trajectories which have started on some surface  $S(x, y, z) = S_0$  at right angles to this surface. In geometrical optics this surface can be considered as a wave-front, and it can then be shown that the pencil of trajectories will be everywhere at right angles to a family of surfaces S(x, y, z) = constant; this is the theorem of Malus and Dupin (§3.3.3).

A certain property of 'transversality' exists also in the general case, as shown in  $\S2$  and  $\S3$  of Appendix I, but its meaning is less simple than in the Malus-Dupin theorem. What remains at right angles to a family of surfaces S = constant is not the unit vector  $\mathbf{s}$  in the direction of the trajectories, but the momentum  $\mathbf{p}$ . As the vector potential is defined only up to a gauge transformation, there exists an infinity of families of transversal surfaces, but in the presence of a magnetic field these cannot be made transversal to the trajectories by any gauge-normalizing procedure.

In the language of geometry, two-dimensional pencils of curves which are at right angles to a family of surfaces form a 'normal congruence,' otherwise they form a 'skew congruence' (see §3.2.3). In light optics and in electrostatic electron optics the trajectories can be ordered in normal congruences, and the surfaces transversal to these are identified with the 'wave-fronts.' In magnetic fields the two-dimensional pencils of trajectories, usually called 'beams,' form skew congruences, and the concept of

<sup>\*</sup> This has been particularly emphasized by W. Ehrenberg and R. E. Siday, *Proc. Phys. Soc.*, B, **62** (1949), 8, who have also pointed out the interesting fact that unless the magnetic field vanishes everywhere it is not possible to normalize **A** by a gauge transformation in such a way that it vanishes with the magnetic field.

transversal wave-fronts cannot be applied to them. This is a rather essential difference between electron optics and light optics.

### 3 Wave mechanics of free electrons

The dual nature of light was first conjectured by Einstein in 1905. Light propagates as if it were an electromagnetic wave, but it interacts with matter as if its energy were concentrated in photons, each with an energy quantum. Soon afterwards Einstein's conjecture was brilliantly verified by observations on photoelectrical and photochemical processes.

The dual conception of material particles is due to Louis de Broglie, who showed in 1923 that if there is a wavelength to be associated, in a relativistically invariant way, with a particle having a mechanical momentum  $p_m$ , this could only be of the form

$$\lambda = \frac{h}{p_m},\tag{18}$$

where h is a universal constant with the dimension of an action, which de Broglie identified with Planck's constant.

Soon afterwards Heisenberg, Born and Jordan developed, quite independently of de Broglie, the first complete mathematical formulation of quantum mechanics, but their methods are less convenient for the discussion of free particles than Schrödinger's wave mechanics, which will now be briefly outlined.

Schrödinger combined de Broglie's ideas with Hamilton's, and was led to the problem of a wave description of particle motion, which stands in the same relation to the dynamics of mass points as wave optics is to geometrical optics. His historical approach, which as we now know is correct only to a certain point, involved of course a certain amount of guessing because, though geometrical optics is logically contained in wave optics, the converse is not true.

Assume that there exists a wave field, whose intensity indicates the density of electrons in a similar way as the intensity of the electromagnetic field indicates the photon density. Moreover, assume that this is a scalar field, whose amplitude is represented by some scalar function  $\Psi(x, y, z, t)$ ; in order to account for its presumed wave-like properties, assume that it satisfies a wave equation

$$\nabla^2 \Psi = \frac{1}{u^2} \ddot{\Psi},$$

u being the wave velocity — in general a function of position. This, of course, is a highly restrictive hypothesis, because the ordinary wave equation with constant velocity of propagation can be generalized in many different ways, of which this is only one, and the simplest.

Substituting for  $\Psi$  a 'monochromatic' wave

$$\Psi(x, y, z, t) = \psi(x, y, z)e^{-i\omega t}$$

we obtain a time-independent equation

$$\nabla^2 \psi = -\left(\frac{\omega}{u}\right)^2 \psi$$
$$= -\left(\frac{2\pi}{\lambda}\right)^2 \psi, \tag{19}$$

in which only the wavelength  $\lambda$  occurs, but not the wave velocity. Assume now that  $\lambda$  is identical with the de Broglie wavelength, if one substitutes for the momentum  $p_m$  the value which a particle would possess at the point x, y, z according to classical mechanics. This can be calculated from (6). For simplicity consider a slow electron in an electrostatic field. In this case de Broglie's relation (18) combined with (6) gives

$$\lambda = \frac{h}{\sqrt{2m(E - e\phi)}}. (20)$$

Substituting this into (19) we obtain

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - e\phi) \psi = 0.$$
 (21)

This is Schrödinger's wave equation for a free particle in a scalar potential field. As it is a time-independent equation, we can interpret it as describing the stationary, e.g. periodic motion of a particle in a field of force. But we can equally apply it to the stationary beams with which we deal in electron optics, in which many particles appear, one after the other, but all under identical conditions. In either case, it appears reasonable to assume, in accordance with Born's statistical interpretation, that the absolute square of the amplitude  $|\psi|^2 = \psi \psi^*$  is proportional to the particle density at the point x, y, z, measured over long times; or, what is the same in this case, that it is proportional to the probability that a particle will be observed at this spot at any instant.

The first verification of (21) was carried out by Schrödinger, who showed that it accounted for the atomic spectra if one assumed that the electron was bound in a field of force which was the same as in the old atom model of Rutherford and Bohr. More relevant for the present purposes was its verification in the case of free electrons, in the discovery of electron diffraction by Davisson and Germer, and independently by G. P. Thomson in 1927–1928.

For slow electrons with a kinetic energy equivalent to eV electron volts, de Broglie's relation (18) gives a wavelength of approximately

$$\lambda = \sqrt{\frac{150}{V}}$$
 ångstrom units.

Thus the wavelength of electrons which can be easily handled in laboratory experiments is of the order of fractions of an ångstrom, of the same order of magnitude as X-ray wavelengths. Hence the wave behaviour of free electrons can be most easily demonstrated in experiments similar to X-ray diffraction in crystal lattices.

The terminology of X-ray analysis, which was also applied to electrons, is somewhat different from that of light optics. What is called X-ray or electron diffraction is really the interference of coherent secondary wavelets emitted by the more or less regularly arranged atoms in a lattice. Diffraction of electrons in the optical sense, by relatively

large material obstacles, whose atomic structure does not come into play, results in extremely small diffraction angles, and was first observed by H. Boersch, in 1940 in an electron microscope.\*

#### 4 The application of optical principles to electron optics

This elementary and incomplete sketch of wave mechanics is sufficient for almost all practical purposes of electron optics. It is not even necessary to make use of the extension of wave mechanics to magnetic fields, because in electron optics it is never necessary to go beyond Kirchhoff's approximation in diffraction problems. The assumptions on which this approximation is based are fully justified in electron optics. With the exception of the fields inside and in the immediate neighbourhood of atomic nuclei, there exist no electric fields which are so abrupt that they change appreciably within a wavelength of the electrons used in electron optics. This is *a fortiori* true for magnetic fields, and the specifically magnetic diffraction effects, which can be inferred from the Klein–Gordon or Dirac wave equation, are far too small to be detected in experiments with free electrons. Thus, with a certain caution which will be explained below, one can safely apply Kirchhoff's diffraction theory (§8.3) which, in its somewhat extended form, may be summarized as follows:

- I. Construct the wave-front from the source to the obstacle or object by measuring equal optical lengths along the rays as calculated by the rules of geometrical optics.
- II. If the obstacle is a dark screen, consider the free part of the wave-front as undisturbed, in phase and in amplitude, and the rest as cut off. In the case of a partially transmitting object, trace the rays through it by the laws of geometrical optics, with the changes in phase and in intensity as determined by its complex refractive index. This is justified in all practical cases because the objects which one considers, e.g. in a microscope, have such small depth that diffraction effects inside them can be safely neglected.

III. In order to calculate the diffraction effects at some remote point, for instance in an optical image, calculate, by the rules of geometrical optics, the transmission between this point and each element of the wave-front emerging from the object or obstacle, and sum the complex amplitudes, taking into account the inclination factors.

Kirchhoff's method, as outlined, can be transferred without modification to electron optics if only electric fields are present, including the strong microscopic fields due to the atomic structure of solid matter, which are predominantly electric. If, however, magnetic fields are present, the wave-fronts can no longer be determined by plotting equal numbers of de Broglie wavelengths along the trajectories. As has been pointed out at the end of §3 of this appendix, the wave-fronts in magnetic fields are no longer orthogonal to the trajectories, but to the lines of total momentum or 'p-lines,' which have no simple geometric-optical interpretation. In principle one could determine the wave-fronts by starting from some given wave-front, and plotting optical lengths along the p-lines. Practically this method is almost useless, because it gives the phases, but not the amplitudes. In practice one is able to avoid this complication, by the artifice of imagining the magnetic lenses replaced by equivalent electric lenses, which produce

<sup>\*</sup> H. Boersch, *Naturwissenschaften*, **28** (1940), 709. Boersch's diffraction photographs are reproduced in W. Glaser, *Grundlagen der Elektronenoptik* (Vienna, Springer, 1952), p. 548.

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the same image field, apart from a rotation of the image as a whole, and a certain rotational distortion of the image. By ignoring these specifically magnetic effects in the propagation process, and adding them only at the end, one can safely apply Kirchhoff's method, and obtain results which are sufficient for all practical purposes.

Though electron optics has the same general mathematical foundation as light optics, its practical structure is very different. Practical light optics has developed on the technical basis of grinding and polishing suitably shaped surfaces on transparent or reflecting solid media. In electron optics there is only one medium: the electromagnetic field. This has its limitations when it comes to the correction of aberrations, especially as space charges and space currents cannot be used for practical reasons. It was discovered early in the development of electron optics that it was impossible to construct diverging lenses and systems free from spherical or from chromatic aberrations, so long as one considered rotationally symmetrical fields only. This led to the development of systems without rotational symmetry, in which these limitations do not hold, and also to systems with curved optic axes, which are almost unknown in light optics. Hence knowledge of optical instruments and design principles is useful in electron optics only in so far as it may pose problems and encourage inventions; the realizations are bound to be widely divergent. On the other hand optical thinking, based on the fundamental analogy of the two fields is likely to be as useful in the future as it was in the first quarter-century of electron optics.