
General Properties of the Electron

Elementary particles exhibit a wave and a particle nature depending on the specific experiment. Owing to its relatively small rest energy $E_0 = m_e c^2 \approx 0.51 \text{ MeV}$, the electron approaches roughly half the speed of light $c \approx 3 \times 10^8 \text{ m s}^{-1}$ at an accelerating voltage $U \approx 60 \text{ kV}$. Therefore, it is necessary to consider relativistic effects for accelerating voltages larger than about 100 kV . Despite the fact that we can consider the electron as a *point-like* particle, it has an angular momentum associated with a magnetic moment:

$$\mu = \frac{eg\mu_0}{2m_e}s = \frac{e\mu_0\hbar}{2m_e}. \quad (2.1)$$

Here, e and \hbar are the charge of the electron and the Planck constant, respectively; μ_0 is the permeability of the vacuum. We use SI units, which now are universally accepted. From the point of view of classical electrodynamics, a magnetic moment originates from a rotating charge of finite extension forming a magnetic dipole. However, the measured ratio of the magnetic moment and the angular momentum or spin $s = \hbar/2$ of the electron is twice as large as predicted by classical electrodynamics. This discrepancy, which requires an empirical *Lande factor* $g = 2$, can only be explained by means of the relativistic electron theory of Dirac [35, 36]. The spin s of the electron is comparable with the *polarization* of the light.

2.1 Particle Nature of the Electron

Within the frame of geometrical charged-particle optics, one considers the electron as a point-like charged mass, whose motion is governed by the laws of *classical mechanics* [37]. We do not consider the *precession* of the electron spin because it does not appreciably affect the motion and we do not consider polarized electron beams. Nevertheless, we can take into account the spin precession sufficiently accurate by means of the so-called *BMT equation* without the need of quantum-mechanical calculations [38].

2.1.1 Equation of Motion

The Lorentz force [37] determines the motion of a particle with charge q in an external electromagnetic field:

$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}). \quad (2.2)$$

Here, \vec{E} and \vec{B} are the electric field strength and the magnetic induction, respectively. The magnetic force vanishes if the velocity \vec{v} of the particle is parallel to the direction of the magnetic induction. According to Newton's law, the force acting on the particle is equal to the temporal change of its kinetic momentum $\vec{p}_k = m\vec{v}$:

$$\frac{d\vec{p}_k}{dt} = \frac{d(m\vec{v})}{dt} = q(\vec{E} + \vec{v} \times \vec{B}), \quad (2.3)$$

$$m = \gamma m_e, \quad \gamma = \frac{1}{\sqrt{1 - \beta^2}}. \quad (2.4)$$

The mass m of the electron is proportional to the relativistic factor γ , which depends on the relative particle velocity $\beta = \vec{v}/c$. Accordingly, the kinetic momentum increases very strongly if the velocity of the particle approaches that of light. The equation of motion is valid only if the particle propagates in vacuum where it does not collide with other particles. To realize approximately this ideal situation, the distance along which the particle travels must be smaller than the mean free path length within the residual gas. Unfortunately, (2.2) can be solved analytically only in rather trivial cases.

To obtain an insight in the general properties of the particle motion, it is advantageous to solve the equation approximately for specific configurations of the electrodes and magnets, which produce the external fields. The development of such calculation procedures is the main task of geometrical charged-particle optics. However, we face in almost all cases the inverse problem to find the electromagnetic field, which affects the path of the particles in a distinct way. Then, it is necessary to find calculation procedures, which yield information on the required course of the trajectories and the geometry and arrangement of the field-producing electrodes and pole pieces.

2.1.2 Conservation of Energy

The electromagnetic field of most electron-optical devices does not depend on time. In this case, we can readily obtain a *first integral* of the second-order differential equation (2.3) by scalar multiplication with the differential path length $d\vec{r} = \vec{v}dt$ and subsequent integration over t , giving

$$\int_{t_0}^t \frac{d(m\vec{v})}{dt} \vec{v} dt = \int_{v_0}^v \vec{v} d(m\vec{v}) = -e \int_{\vec{r}_0}^{\vec{r}} \vec{E} d\vec{r}. \quad (2.5)$$

The magnetic term of the Lorentz force does not contribute because it is perpendicular to the velocity.

In the case of stationary magnetic fields ($\partial \vec{A}/\partial t = 0$), we can readily evaluate the last integral by employing the relation

$$\vec{E} = -\text{grad } \varphi - \dot{\vec{A}} = -\text{grad } \varphi. \quad (2.6)$$

The resulting voltage $U = \varphi - \varphi_0$ is the difference between the electric potential φ at the point of observation \vec{r} and the potential φ_0 at the initial point \vec{r}_0 . We can also evaluate analytically the second integral in (2.5) by partial integration, yielding

$$\begin{aligned} \int \vec{v} d(m\vec{v}) &= m\vec{v}^2 - \int m\vec{v} d\vec{v} = m\vec{v}^2 - \frac{m_e c^2}{2} \int \frac{d(\beta^2)}{\sqrt{1-\beta^2}} \\ &= m\vec{v}^2 + m_e c^2 \sqrt{1-\beta^2} = \frac{m_e c^2}{\sqrt{1-\beta^2}} = mc^2. \end{aligned} \quad (2.7)$$

By inserting this result into (2.5) and considering (2.6), we obtain the conservation of energy in the relativistic form

$$E = E_0 + E_k + E_p = m_e c^2 + (m - m_e) c^2 - e\varphi = mc^2 - e\varphi = m_0 c^2 - e\varphi_0 = \text{const.} \quad (2.8)$$

The index 0 indicates the value taken at the initial position \vec{r}_0 . We should not confuse the symbol E for the energy with the vector symbol \vec{E} for the electric field strength. The potential energy $E_p = -e\varphi$ is not a measurable quantity because the electric potential is not gauge invariant. The kinetic energy $E_k = (m - m_e) c^2$ approaches the classic expression $m_e \vec{v}^2/2$ in the nonrelativistic limit $\beta \rightarrow 0$.

In the following, we use the gauge such that $\varphi_0 = 0$ at the surface of the cathode where $\vec{v}_0 = 0$. Then, the potential at the point of observation is identical with the voltage U applied between this point and the cathode. Moreover, the constant on the right-hand side adopts the value $\text{const.} = E_0 = m_e c^2$, which coincides with the rest energy E_0 of the electron. In this case, we derive from (2.8) for the velocity v and the kinetic momentum p_k of the electron the expressions

$$v = c \sqrt{\frac{2eU}{E_0} \frac{\sqrt{1 + eU/2E_0}}{1 + eU/E_0}}, \quad p_k = mv = \frac{eU}{c} \sqrt{1 + \frac{2E_0}{eU}}, \quad \gamma = \frac{m}{m_e} = 1 + \frac{eU}{E_0}. \quad (2.9)$$

At the limit $eU \gg E_0$, the velocity approaches the velocity of light c . Any further acceleration increases only the mass and the kinetic momentum in proportion to U (Fig. 2.1).

2.1.3 Hamilton's Principle

We can also derive the Newtonian path equation (2.3) from *Hamilton's principle* of classical mechanics [39]. Hamilton demonstrated that it is possible

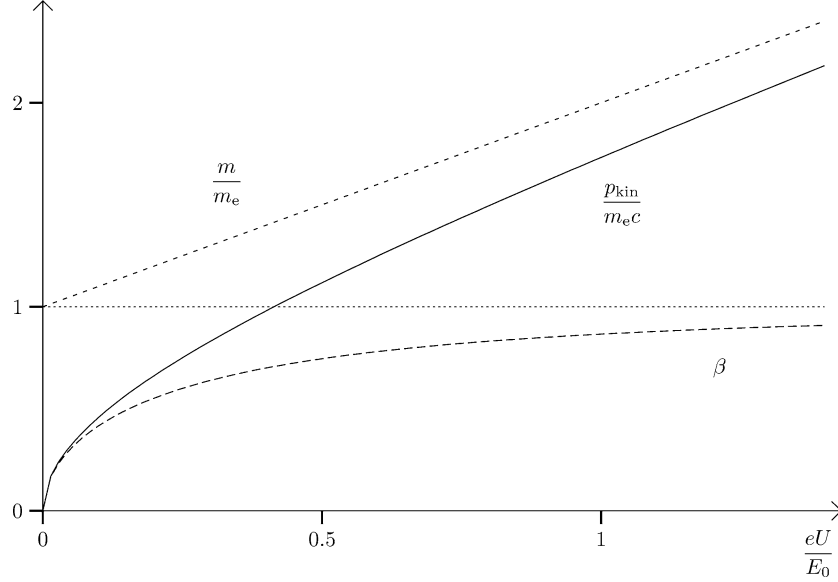


Fig. 2.1. Normalized mass $m/m_e = \gamma$, relative velocity $\beta = v/c$, and normalized kinetic momentum $p_k/m_e c$ as functions of the normalized kinetic energy eU/E_0

to obtain the optical laws from a single characteristic function, which one later called *eikonal*, derived from the Greek word $\epsilon\iota\kappa\omicron\nu$ (icon) meaning image [40]. Hamilton himself showed that the techniques he had developed for handling optical problems are also applicable in mechanics. This is the reason why it is advantageous to treat many problems of charged-particle optics most effectively by means of the eikonal method. We obtain this function most conveniently by employing Hamilton's principle. It states that the true path $\vec{r} = \vec{r}(t)$ of a particle traveling from the initial point \vec{r}_0 at time t_0 to the point \vec{r} makes the *action*

$$W = W(\vec{r}, t; \vec{r}_0, t_0) = \text{Ex} \int_{t_0}^t L(\vec{r}', \dot{\vec{r}}', t') dt' \quad (2.10)$$

an *extremum*. It is a minimum if the point of observation \vec{r} is located in front of the caustic formed by the loci of the points of intersection of adjacent trajectories starting from the common origin \vec{r}_0 . However, the action may adopt a maximum if the caustic is located between the origin and the point of observation. The caustic can degenerate to a point, which represents the so-called *conjugate* point with respect to the origin \vec{r}_0 . If we can achieve this condition for all points of a given object plane, we obtain a perfect image of this plane at the corresponding conjugate image plane.

The Lagrangian L , which is a function of the position and the velocity $\vec{v} = \dot{\vec{r}}$ of the particle, must be a *Lorentz-invariant* scalar quantity since we

consider relativistic particles. In the classical case, the *Lagrangian* is the difference between the kinetic energy and the potential energy. To obtain a *covariant* expression for L , we assume the simple case that it is a scalar product of two 4-vectors, one of which is the path length element. To avoid the use of metric coefficients, we describe the 4-vectors in Minkowski space. In this case, we have a four-dimensional *pseudo-Euclidian* space where the fourth (time-like) component of any 4-vector is purely imaginary. For example, the four-dimensional position vector has the form $\vec{R} = (x, y, z, ict)$. Using this representation, we obtain for the components of the four-dimensional differential path length element the expressions

$$dx_1 = dx, \quad dx_2 = dy, \quad dx_3 = dz, \quad dx_4 = ic dt. \quad (2.11)$$

To obtain an action, the other 4-vector must have the dimension of a momentum. The appropriate vector is the *canonical momentum* 4-vector $\vec{P} = (\vec{p}, p_4)$ with the spatial component

$$\vec{p} = m\vec{v} - e\vec{A}, \quad (2.12)$$

where \vec{A} is the magnetic vector potential, and the *time-like* imaginary component

$$p_4 = m\dot{x}_4 - eA_4 = i(mc - e\varphi/c) = iE/c. \quad (2.13)$$

The comparison of this result with (2.8) shows that the fourth component of the canonical momentum represents the energy up to the imaginary factor i/c . Scalar multiplication of the canonical momentum 4-vector with the velocity 4-vector yields the Lagrangian in covariant form

$$L = \sum_{\mu=1}^4 p_{\mu} \frac{dx_{\mu}}{dt} = m(\vec{v}^2 - c^2) - e\vec{v}\vec{A} + e\varphi = -m_e c^2 \sqrt{1 - \beta^2} + e\varphi - e\vec{v}\vec{A}. \quad (2.14)$$

We can readily verify the correctness of this Lagrangian by means of the *Euler-Lagrange* equations:

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}_{\mu}} \right) - \frac{\partial L}{\partial x_{\mu}} = 0, \quad \mu = 1, 2, 3. \quad (2.15)$$

We derive these equations from the action function (2.10) by employing the condition $\delta W = 0$ and by keeping the initial and final positions fixed ($\delta \vec{r}_0 = 0, \delta \vec{r} = 0$). By inserting (2.14) for L into (2.15), we eventually obtain the path equation (2.3). Hence, we can readily determine the action function W if we insert the solutions of this equation in the integrand (2.14) of the integral (2.10) and perform the integration with respect to the independent time variable.

If we vary slightly the coordinates of the point of observation by $\delta \vec{r}$ and the time of observation by δt , we change the path of the particle to a neighboring trajectory starting from the fixed origin \vec{r}_0 . As a result, the action changes by

$$\delta W = W(\vec{r} + \delta\vec{r}, t + \delta t; \vec{r}_0, t_0) - W(\vec{r}, t; \vec{r}_0, t_0) = \sum_{\mu=1}^4 p_{\mu} \delta x_{\mu}. \quad (2.16)$$

Since we can perform the infinitesimal displacement arbitrarily, we select any one of the four infinitesimal displacements δx_{μ} as nonzero, resulting in

$$\frac{\partial W}{\partial x_{\mu}} = p_{\mu} = m\dot{x}_{\mu} - eA_{\mu} \Rightarrow \frac{\partial W}{\partial x_{\mu}} + eA_{\mu} = m\dot{x}_{\mu}. \quad (2.17)$$

Summation of the squares of the second relation yields the *relativistic Hamilton–Jacobi equation* for the electron:

$$\sum_{\mu=1}^4 m^2 \dot{x}_{\mu}^2 = \sum_{\mu=1}^4 (p_{\mu} + eA_{\mu})^2 = \sum_{\mu=1}^4 \left(\frac{\partial W}{\partial x_{\mu}} + eA_{\mu} \right)^2 = m_e^2 \frac{\vec{v}^2 - c^2}{1 - \vec{v}^2/c^2} = -m_e^2 c^2. \quad (2.18)$$

To separate the time-like component from the spatial components, we rewrite the equation in the form

$$(\vec{\nabla}W + e\vec{A})^2 - \frac{1}{c^2} \left(\frac{\partial W}{\partial t} - e\varphi \right)^2 + m_e^2 c^2 = 0. \quad (2.19)$$

Contrary to the Hamilton–Jacobi equation of classical mechanics, (2.19) is of second degree in the time derivative of the action function W . This behavior results from the condition that the relativistic correct equations must be Lorentz invariant.

A constant action $W = W(\vec{r}, t; \vec{r}_0, t_0) = W_0$ represents a hypersurface in four-dimensional space. We can depict this surface approximately by a discrete set of surfaces $W_n = W(\vec{r}, n\Delta t, \vec{r}_0) = W_0$, $n = 1, 2, \dots$, in the conventional three-dimensional space. If both the magnetic vector potential \vec{A} and the electric potential φ do not depend on the time t , the action function decomposes as

$$W(\vec{r}, t; \vec{r}_0, t_0) = S(\vec{r}, \vec{r}_0, E) + E(t - t_0). \quad (2.20)$$

The *reduced action* or *eikonal* S is a function of the position coordinates and the energy E . By inserting the relation (2.20) into (2.19) and choosing the gauge for φ such that $E = E_0 = m_e c^2$, we obtain the so-called *eikonal equation* of the electron:

$$(\vec{\nabla}S + e\vec{A})^2 = m^2 v^2 = 2m_e e \varphi^*. \quad (2.21)$$

Here, $\vec{\nabla} = \text{grad}$ is the *nabla* operator. For reasons of simplicity, we have introduced the *relativistic modified* electric potential:

$$\varphi^* = \varphi \left(1 + \frac{e\varphi}{2m_e c^2} \right) \approx \varphi \left(1 + \frac{e\varphi}{1.02 \text{ MeV}} \right). \quad (2.22)$$

The eikonal represents a characteristic function, which governs the imaging properties of the optical system. This function has the properties of an optical potential.

2.1.4 Principle of Maupertuis

The *principle of Maupertuis* or *principle of least action* is the special case of Hamilton's principle for *conservative* systems. Since the action can also be a maximum, it is more appropriate to use the expression "principle of stationary action." For conservative systems, the total energy $E = -ip_4c = mc^2$ is constant. As a result, the action (2.10) adopts the form

$$W = \text{Ex} \sum_{\mu=1}^4 \int_{\vec{R}_0}^{\vec{R}} p_\mu dx_\mu = \text{Ex} \int_{\vec{r}_0}^{\vec{r}} \vec{p} d\vec{r} + p_4(x_4 - x_{40}) = S - E(t - t_0), \quad (2.23)$$

where $\vec{R} = (\vec{r}, ict)$ denotes the four-dimensional position vector. It readily follows from the relations (2.23) that the reduced action or eikonal

$$S = S(\vec{r}, \vec{r}_0, E) = \text{Ex} \int_{\vec{r}_0}^{\vec{r}} \vec{p} d\vec{r} \quad (2.24)$$

is also an extremum. This finding is Maupertuis' principle, which we may also write as

$$\delta S = \delta \int_{\vec{r}_0}^{\vec{r}} (m\vec{v} - e\vec{A}) d\vec{r} = 0. \quad (2.25)$$

To derive the corresponding Euler-Lagrange equations, we must fix the origin \vec{r}_0 and the point of observation \vec{r} . If we vary the coordinates of the position vector \vec{r} , we readily obtain the relation

$$\vec{\nabla} S + e\vec{A} = m\vec{v}. \quad (2.26)$$

Hence, the direction of the particle velocity \vec{v} is perpendicular to the surfaces of constant reduced action

$$S_\nu(\vec{r}, \vec{r}_0, E) = E(t_\nu - t_0), \quad \nu = 1, 2, \dots, \quad (2.27)$$

only in the absence of a magnetic field ($\vec{A} = 0$), as illustrated in Fig. 2.2. We can interpret the continuous set of wave surfaces (2.27) as a sequence of instant photographs of the propagating discontinuity surface $W = 0$, which are taken at regular intervals of time. The external fields may deform this surface considerably, but they can never tear it into pieces. In the presence of a magnetic field, the actual paths of the particles do *not* coincide with orthogonal trajectories.

By taking the square of the relation (2.26), we readily derive the eikonal equation (2.21). The eikonal equation (2.24) describes the propagation of an *ensemble* of charged particles, which originate from a common point source.

2.1.5 Time of Flight

We define the time of flight $T = t - t_0$ as the time, which the particle needs to travel from its origin \vec{r}_0 at time t_0 to the point of observation \vec{r} . For reasons of simplicity, we assume stationary electromagnetic fields.

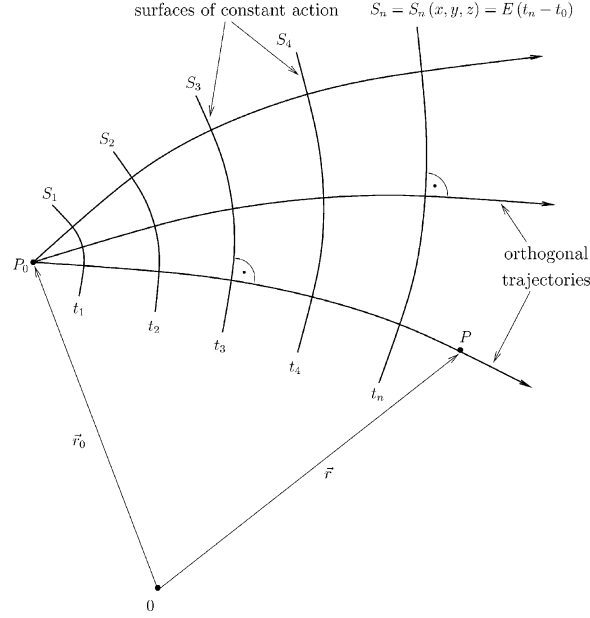


Fig. 2.2. Homocentric paths of electrons in the case $\vec{A} = 0$, $\varphi \neq 0$ representing the orthogonal trajectories of the set of surfaces of constant reduced action $S_\nu = S_\nu(\vec{r}, \vec{r}_0; E) = E(t_\nu - t_0)$

In this case, we obtain from (2.8) the expression

$$v = \frac{ds}{dt} = c \sqrt{1 - \frac{E_0^2}{(E + e\varphi)^2}}. \quad (2.28)$$

Here, $ds = |d\vec{r}|$ is the differential path length element. The integration of the differential equation (2.28) along the particle trajectory from its origin to its endpoint yields directly the time of flight:

$$T = \frac{1}{c} \int_{\vec{r}_0}^{\vec{r}} \frac{E + e\varphi}{\sqrt{(E + e\varphi)^2 - E_0^2}} ds = \frac{\partial S}{\partial E}. \quad (2.29)$$

By differentiating (2.27) with respect to the total energy E and putting $t_\nu = t$, we readily obtain the second relation in (2.29).

2.2 Wave Properties of the Electron

Already in 1828, *Hamilton* discovered the close connection existing between the laws of geometrical light optics and the laws of classical mechanics. He showed that the techniques, which he had developed for handling optical

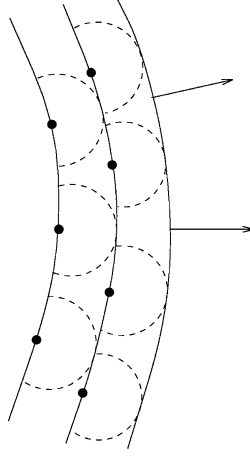


Fig. 2.3. Huyghens' principle

problems, are also very useful in mechanics. Today, these methods play a central role in analytical mechanics and quantum mechanics, while they are almost forgotten in light optics. *Newton* assumed that light consists of tiny particles, while *Huyghens* postulated that light is a wave phenomenon. Moreover, Huyghens demonstrated, in 1690, that one could derive the concept of a *light ray* from the wave formalism without any contradictions. According to Huyghens' principle, each point of a wave surface at time t_0 acts as a source of an elementary wave. This wave is a spherical wave in the field-free region, as shown in Fig. 2.3. The summation of these waves performed at some later time $t = t_0 + \Delta t$ yields the new wave surface, which is the envelope of all elementary waves. The contributions of the backward propagating parts of the elementary waves cancel out by interference. The light rays are the orthogonal trajectories of the set of envelopes formed at times $t_\nu = t_0 + \nu \Delta t$, $\nu = 1, 2, \dots$. The wave description also accounts for diffraction effects, which one cannot explain in the frame of geometrical optics, which represents an approximation for the limit of very short wavelengths ($\lambda \rightarrow 0$).

According to the hypothesis of de Broglie [2], the electron has a particle and a wave property. We can consider this duality by means of a wave formalism in close relation to that of light. On account of this analogy, de Broglie postulated that the Einstein relation

$$E = h\nu = \hbar\omega \quad (2.30)$$

is also valid for the electron. By attributing a frequency $\nu = \omega/2\pi$ and a wavelength $\lambda = 2\pi/k$ to the electron, de Broglie derived that the equivalent relation

$$\vec{p} = \hbar\vec{k} \quad (2.31)$$

exists between the canonical momentum \vec{p} and the wave vector \vec{k} . By defining $k_4 = i\omega/c$ as the time-like component of a wave 4-vector $\vec{K} = (\vec{k}, k_4)$, we can

write (2.30) and (2.31) as a single relativistic *covariant* equation

$$\vec{P} = \hbar \vec{K}. \quad (2.32)$$

Hence, a matter wave with wave 4-vector \vec{K} is attributed to an elementary particle with a canonical momentum 4-vector \vec{P} .

2.2.1 Eikonal and Fermat's Principle

The Hamilton–Jacobi equation is most appropriate for incorporating the wave nature of the electron. According to the rules of quantum mechanics, we must consider the components of the canonical momentum 4-vector as gradient operators

$$p_\mu = \frac{\hbar}{i} \frac{\partial}{\partial x_\mu}, \quad (2.33)$$

which act on the wave function $\psi_e = \psi_e(x_\mu) = \psi_e(\vec{r}, t)$. If we neglect the effect of the spin, the wave function is a single component complex function. By substituting (2.33) for p_μ in the Hamilton–Jacobi equation (2.18), we readily obtain the *Klein–Gordon equation*:

$$\sum_{\mu=1}^4 \left(\frac{\hbar}{i} \frac{\partial}{\partial x_\mu} + eA_\mu \right)^2 \psi_e + m_e^2 c^2 \psi_e = 0. \quad (2.34)$$

This four-dimensional wave equation describes correctly the relativistic motion of the electron if we ignore the negligibly small effect of the spin. In the absence of external fields ($A_\mu = 0$), the solutions are plane waves of the form

$$\psi_e = \psi_{e0} e^{iW/\hbar}. \quad (2.35)$$

The phase $W/\hbar = \Omega$ is the Lorentz-invariant scalar product formed by the four-dimensional position vector $\vec{R} = (\vec{r}, ict)$ and the wave 4-vector $\vec{K} = (\vec{k}, k_4 = i\omega/c)$, giving

$$W/\hbar = \sum_{\mu} x_\mu p_{k\mu}/\hbar = \sum_{\mu} k_\mu x_\mu = \vec{k}\vec{r} - \omega t. \quad (2.36)$$

By inserting the solution into (2.34), we obtain the conservation of energy:

$$\hbar^2 (\vec{k}^2 - \omega^2/c^2) + m_e^2 c^2 = m^2 \vec{v}^2 - E^2/c^2 + E_0^2 = 0. \quad (2.37)$$

Here, we do not need to employ the gauge

$$\varphi = -icA_4 = 0, \quad \text{for } \vec{v} = 0. \quad (2.38)$$

To derive the eikonal equation (2.21), we assume stationary fields. Moreover, the form (2.35) of the field-free solution suggests the *WKB* ansatz:

$$\psi_e = \psi_{e0} e^{i(S-Et)/\hbar}, \quad (2.39)$$

where $S = S(\vec{r})$ is a function of the position \vec{r} of the electron. The WKB approximation of quantum mechanics is equivalent to the much older eikonal approximation of light optics. By inserting the ansatz (2.39) into the wave equation (2.34) and employing both the gauge (2.38) and the Lorentz gauge

$$\sum_{\mu=1}^4 \frac{\partial A_\mu}{\partial x_\mu} = \text{div } \vec{A} + \dot{\varphi}/c^2 = 0, \quad (2.40)$$

we eventually obtain

$$-i\hbar\Delta S + (\vec{\nabla}S + e\vec{A})^2 - 2m_e e\varphi^* = 0. \quad (2.41)$$

Here, $\Delta = \vec{\nabla}^2$ is the *Laplace operator*. In the classical limit $\hbar \rightarrow 0$, (2.41) reduces to the eikonal equation:

$$(\vec{\nabla}S + e\vec{A})^2 = 2m_e e\varphi^*. \quad (2.21)$$

The solution of the eikonal equation (2.21) satisfies *Fermat's principle* (Fermat, 1679), which states that the optical path $L = S/q_0$ between the origin \vec{r}_0 and the point of observation \vec{r} is an extremum:

$$L = S/q_0 = \text{Ex} \int_{\vec{r}_0}^{\vec{r}} n(\vec{r}) d\vec{s} = \frac{1}{k_0} \int_{\vec{r}_0}^{\vec{r}} \vec{k} d\vec{r}. \quad (2.42)$$

The use of variational principles dates back to the earliest Greek philosophers. They derived them on ground of their aesthetic and metaphysical ideal of simplicity for the laws of nature. Hero of Alexandria (125 BC) made the first rigorous use of an optical variational principle when he proved that for a mirror, the angle of incidence equals the angle of reflection. He showed that in this case, the path taken by a ray from the object to the observer is the shortest of all possible paths. Fermat's principle is an extension of this principle for media with spatially varying index of refraction. We have chosen the normalization momentum

$$q_0 = \hbar k_0 = \sqrt{2em_e\Phi_0^*}, \quad (2.43)$$

in such a way that the index of refraction for charged particles

$$n = n(\vec{r}) = k/k_0 = \sqrt{\frac{\varphi^*}{\Phi_0^*}} - \frac{e}{q_0} \vec{A} \vec{e}_t \quad (2.44)$$

is unity in the absence of an electromagnetic field ($\vec{A} = 0$, $\varphi^* = \varphi_0^* = \Phi_0^*$) in the space between the ray-defining points \vec{r} and \vec{r}_0 . Here, Φ denotes the electric potential on the optic axis and $\lambda_0 = 2\pi/k_0$ is the wavelength at the center of the starting plane $z = z_0$.

Our definition of the index of refraction corresponds to that of light optics because the optical path length (2.42) for charged particles degenerates to the geometrical distance $l = |\vec{r} - \vec{r}_0|$ between the ray-defining points in the absence of an electromagnetic field, as it is the case for light rays propagating in vacuum. From the point of view of wave optics, Fermat's principle is a direct consequence of the fact that the light rays are the orthogonal trajectories to the wave surfaces:

$$k_0 l - \omega t = \text{const.} \quad (2.45)$$

To prove this behavior, we consider a set of wave surfaces $l_\nu = l_0 + \nu\lambda$, $\nu = 0, 1, \dots, n$, shown in Fig. 2.4. The separation between any two adjacent wave surfaces is chosen to be equal with the wavelength. We consider an arbitrary path connecting the origin P_0 with the endpoint P , as illustrated by the dashed curve. The solid curve represents the orthogonal trajectory. It readily follows from the figure that we can write the optical path length along the dashed curve as

$$\int_{\vec{r}_0}^{\vec{r}} n \, ds = \frac{1}{k_0} \int_{\vec{r}_0}^{\vec{r}} k \, dz = \lambda_0 \int_{\vec{r}_0}^{\vec{r}} \frac{ds}{\lambda} \approx \lambda_0 \sum_{\nu=1}^n \frac{\Delta s_\nu}{\lambda_\nu} = \sum_{\nu=1}^n \frac{\lambda_0}{\cos \alpha_\nu}. \quad (2.46)$$

This length adopts a minimum if $\alpha_\nu = 0$. Hence, the true path is the trajectory, which is orthogonal to the wave surfaces. The second relation in (2.44) describes this behavior, as can be seen by taking the gradient.

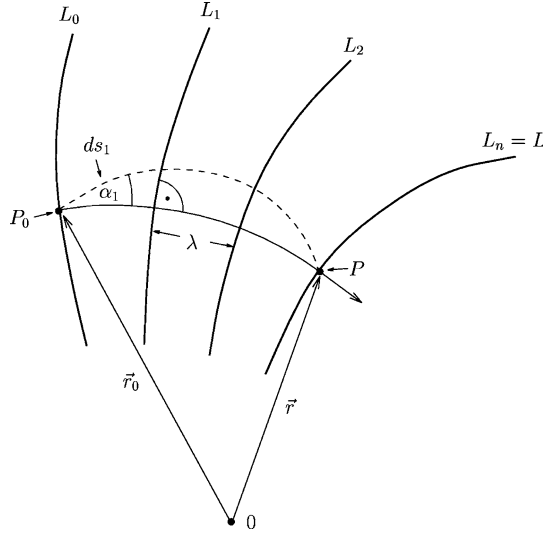


Fig. 2.4. Fermat's principle ($L_n = l_n$)

2.2.2 Phase, Wavelength, Frequency, Phase and Group Velocity, and Index of Refraction

Already in 1828, Hamilton discussed the close “formal” relation between Fermat’s principle of optics and Maupertuis’ principle of mechanics. Owing to Hamilton’s profound knowledge of optics and mechanics, it is very likely that he did not consider this equivalence to be a meaningless coincidence. However, it took almost 200 years until de Broglie postulated that this equivalence is real for elementary particles reflecting the dualism between their wave and particle nature. Accordingly, we postulate as the *phase* of the matter wave

$$\Omega(\vec{r}, t) = \frac{W}{\hbar} = \frac{1}{\hbar} \sum_{\mu=1}^4 \int k_{\mu} dx_{\mu} = \int \vec{k} d\vec{r} - \omega t. \quad (2.47)$$

We know from electron microscopy that the phase of the scattered electron wave contains the information about the atomic structure of the object. Unfortunately, the geometrical path of the electron through the object is difficult to calculate, except for fast electrons passing through very thin objects (few atomic layers). In this special case, the electrons move approximately along straight lines through the object. These conditions are fulfilled in the electron microscope for amorphous objects, which behave like phase objects in light microscopy.

The energy E of a photon is related to its frequency ν by the Einstein relation $E = h\nu$. Both quantities are measurable. This is not the case for electrons and ions because we cannot unambiguously define their energy $E = E_0 + E_{\text{kin}} + E_{\text{pot}}$ since the electric potential φ and the related potential energy E_{pot} are not gauge invariant. Therefore, one can define the frequency of a charged-particle wave only up to an arbitrary constant. As a result, we can only measure differences of frequencies, as it is the case in any interference experiment.

The same behavior holds true for the wave vector $\vec{k} = (m\vec{v} - e\vec{A})/\hbar = \vec{\nabla}S/\hbar$. We cannot measure it because the magnetic vector potential is not gauge invariant. Moreover, we confront the additional difficulty that the direction $\vec{e}_t = \vec{v}/v$ of the particle trajectory is not perpendicular to the wave surfaces in the presence of a magnetic field ($\vec{A} \neq 0$). Hence, the distance between any adjacent wave surfaces S_n and S_{n+1} measured along any trajectory does not represent the shortest distance $2\pi/k = \lambda$, as demonstrated in Fig. 2.5. The distance along the trajectory equals the wavelength λ only in the absence of a magnetic field.

To retain this convention, we define the wavelength of the electron wave in the same way as

$$\lambda = \frac{2\pi}{\vec{k}\vec{e}_t} = \frac{h}{mv - e\vec{A}\vec{e}_t} = \frac{2\pi}{k \cos \alpha}. \quad (2.48)$$

Here, α defines the angle between the direction of the actual path and the direction of the canonical momentum or wave vector. In the absence of a

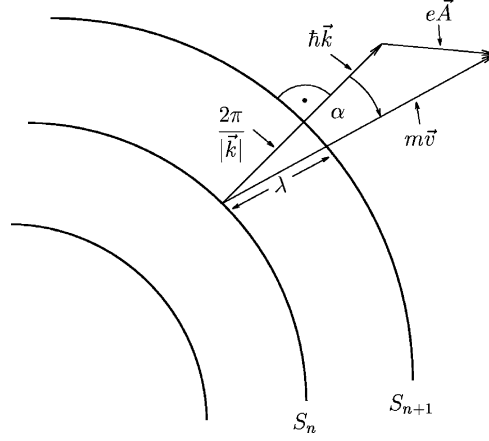


Fig. 2.5. Definition of the wavelength of the electron wave in the presence of a magnetic vector potential

magnetic field ($\vec{A} = 0$), the wavelength

$$\lambda = \frac{h}{mv} = \frac{h}{m_e c} \frac{m_e c}{mv} = \lambda_C \sqrt{\frac{E_0}{2eU^*}} \approx \sqrt{\frac{1.5 \text{ V}}{U^*}} \text{ nm} \quad (2.49)$$

is a measurable quantity because the relativistic modified acceleration voltage $U^* = U(1 + eU/2E_0)$ is gauge invariant; $\lambda_C = 2\pi/k_C = 2.426 \text{ pm}$ denotes the *Compton wavelength*. For an accelerating voltage $U \approx U^* = 150 \text{ V}$ with respect to the cathode potential, the wavelength equals 1 \AA , which is roughly the diameter of a hydrogen atom. Therefore, the resolution limit

$$d \approx \lambda/\theta \quad (2.50)$$

of the electron microscope (EM) is very small. Unfortunately, the spherical aberration of the round lenses limits the maximum usable aperture angle $\theta \approx 0.01$ in conventional EMs. As a result, such EMs cannot achieve sub-Angstrom resolution at voltages below about 1 MV . This behavior is the reason for the ongoing efforts to compensate for the unavoidable chromatic and spherical aberration of round lenses (*Scherzer theorem* [8]) by means of multipole or mirror correctors. We shall treat extensively the different correction methods in Chap. 9.

One characterizes refracting media in light optics by their *index of refraction* $n = \lambda_v/\lambda$. We can use this definition also for the particle wave if we substitute λ_C for the vacuum wavelength λ_v of light. By employing the relation (2.48), we readily obtain the particle-optics index of refraction as

$$n = \frac{\lambda_0}{\lambda} = \frac{m\vec{v} - e\vec{A}\vec{e}_t}{q_0} = \sqrt{\frac{\varphi^*}{\Phi_0^*}} - \frac{e}{q_0} \vec{A}\vec{e}_t. \quad (2.51)$$

In analogy to light optics, the electromagnetic field represents an inhomogeneous *anisotropic* medium of refraction for the charged particles. The anisotropy stems from the directional dependence of n on the direction of flight of the particle in the presence of a magnetic field. Therefore, only electrostatic systems have an *isotropic* index of refraction. Using the terminology of light optics, all electron lenses represent *gradient-index* lenses because the electromagnetic potentials are continuous functions of the spatial coordinates, which cannot change abruptly at a given surface, as does the light-optical index of refraction at the surface of a lens.

The phase (2.47) of the electron wave cannot be measured because each component $k_\mu = (m\dot{x}_\mu - eA_\mu)/\hbar$ of the wave 4-vector depends on the 4-vector potential. Its component A_μ is only determined up to the derivative $\partial\chi/\partial x_\mu$ of an arbitrary scalar function $\chi = \chi(\vec{r}, x_4)$. By introducing this function, we change the gauge of the 4-vector potential (\vec{A} , $A_4 = i\varphi/c$) resulting in the phase

$$\Delta\Omega = \sum_{\mu=1}^4 \int_{x_{\mu 0}}^{x_\mu} \frac{\partial\chi}{\partial x_\mu} dx_\mu = \chi - \chi_0. \quad (2.52)$$

Therefore, it is not possible to measure the absolute phase of the particle wave. This result is plausible because we must measure the phase by an interference experiment, which records phase differences or differences of wave vectors.

The frequency $\nu = \omega/2\pi$ of the electron wave relates to its energy E in the same way as in the case of light:

$$E = \hbar\omega = -icp_4 = -ic(m\dot{x}_4 - eA_4) = (mc^2 - e\varphi). \quad (2.53)$$

By employing the relation

$$\begin{aligned} \frac{1}{\hbar^2} \sum_{\mu=1}^4 m^2 \dot{x}_\mu^2 &= \frac{1}{\hbar^2} \sum_{\mu=1}^4 (p_\mu + eA_\mu)^2 = \sum_{\mu=1}^4 (k_\mu + eA_\mu/\hbar)^2 \\ &= (\vec{k} + e\vec{A}/\hbar)^2 - (\omega + e\varphi/\hbar)^2/c^2 = -k_C^2, \end{aligned} \quad (2.54)$$

the frequency can be expressed in the form of a dispersion relation as

$$\omega = -e\varphi/\hbar + c\sqrt{(\vec{k} + e\vec{A}/\hbar)^2 + k_C^2}. \quad (2.55)$$

Since both the frequency and the wave vector depend on the gauge of the 4-vector potential, the phase velocity $v_p = \omega/k$ is not gauge invariant and, therefore, not measurable. Fortunately, this behavior is of no concern because it is not possible to transfer any information by means of a single monochromatic wave. We can transfer a signal only by means of a wave package formed by a superposition of waves with different wave vectors. This superposition produces a *beat*, which propagates with the measurable *group velocity*:

$$\vec{v}_g = \vec{\nabla}_k \omega = c^2 \frac{\vec{k} + e\vec{A}/\hbar}{\omega + e\varphi/\hbar} = c^2 \frac{m\vec{v}}{mc^2} = \vec{v}. \quad (2.56)$$

The beat of the modulated particle wave propagates with the same measurable velocity as the corpuscular particle. In the presence of a magnetic field ($\vec{A} \neq 0$), the elementary Huyghens' waves are no longer spherical waves. They form elliptical waves in the case of constant vector potential. The corresponding wave surfaces are rotational ellipsoids where one of the two principal axes is located in the direction of the particle trajectory. One of the two focal points of the ellipsoid is located at the origin of the elementary wave. Using these elementary waves, Huyghens' construction of the wave surfaces is also applicable in the presence of an electromagnetic field. In this case, we must choose the distance between neighboring wave surfaces in such a way that the vector potential does not appreciably vary in the region between any two subsequent wave surfaces.

A very instructive example for the influence of the vector potential on the phase of the electron wave is the *Aharonov-Bohm effect* [41]. To demonstrate this effect, we consider the experimental arrangement of Moellenstedt and Dueker [42], as shown in Fig. 2.6. It consists of a positively charged wire, forming an electron-optical biprism, and a bifilar solenoid with an adjustable current placed below the wire. The current produces a magnetic field only

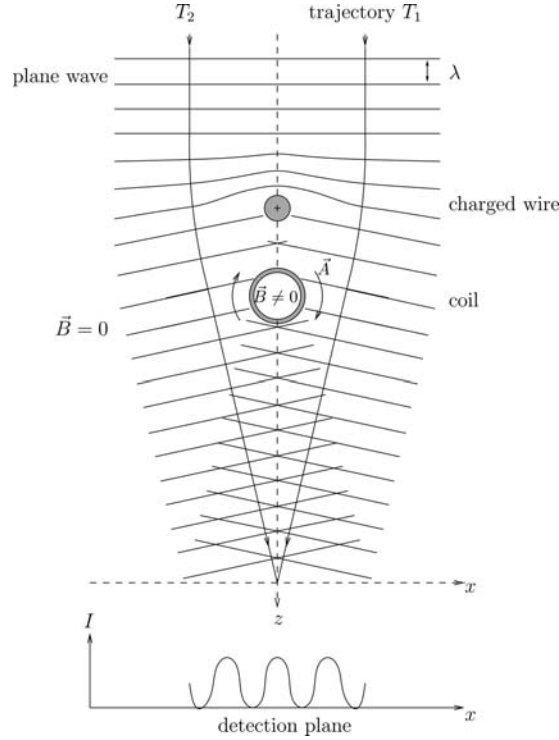


Fig. 2.6. Arrangement of the Moellenstedt's experiment demonstrating the Aharonov-Bohm effect

in the interior of the coil. Although the magnetic field vanishes in the region outside of the coil, the magnetic vector potential does not ($\vec{A} \neq 0$) due to the relation

$$\oint \vec{A} d\vec{s} = \iint (\vec{\nabla} \times \vec{A}) d\vec{\sigma} = \iint \vec{B} d\vec{\sigma} = \Phi_m, \quad (2.57)$$

where $d\vec{\sigma}$ denotes the differential surface element. Since we can choose the closed contour of the line-integral arbitrarily and because the magnetic flux Φ_m varies if the current is changed, the vector potential must change in the entire outer space. Hence, we cannot nullify the vector potential everywhere in this region by means of a gauge.

We further assume a plane wave for the incident electron, whose direction of propagation is parallel to the dashed line through the centers of the wire and the coil. The biprism splits the wave $\psi_e = \psi_{e1} + \psi_{e2}$ into two coherent partial waves:

$$\psi_{e1} = \psi_{e0} e^{i\Omega_1(\vec{r}, t)}, \quad \psi_{e2} = \psi_{e0} e^{i\Omega_2(\vec{r}, t)}, \quad (2.58)$$

which propagate in different directions and interfere in the region beneath the coil. The phases Ω_1 and Ω_2 are imaginary in the region where the intensity of the partial waves is negligibly small. In the detection plane, the overlapping parts of the waves form an interference pattern with intensity:

$$I = \psi_e \bar{\psi} = 2 |\psi_{e0}|^2 [1 + \cos(\Omega_1 - \Omega_2)]. \quad (2.59)$$

The phase difference

$$\begin{aligned} \Delta\Omega &= \Omega_1 - \Omega_2 \\ &= \frac{1}{\hbar} \int_{T_1} (m\vec{v} - e\vec{A}) d\vec{s} - \frac{1}{\hbar} \int_{T_2} (m\vec{v} - e\vec{A}) d\vec{s} = \frac{mv}{\hbar} (l_1 - l_2) + \frac{e}{\hbar} \oint \vec{A} d\vec{s} \\ &= k_0 (l_1 - l_2) + \frac{e\Phi_m}{\hbar} \end{aligned} \quad (2.60)$$

determines the locations of the maxima and zeros of the intensity (2.59).

Electrons attributed to a single plane wave start from a common point source. Therefore, the path lengths l_1 and l_2 of the symmetric trajectories T_1 and T_2 coincide. Hence, the intensity at the center of the detection plane depends only on the magnetic flux within the coil:

$$I = I_0 [1 + \cos(e\Phi_m/\hbar)]. \quad (2.61)$$

Moellenstedt's experiment proves convincingly that the fringes move when the current is changed. This change alters the phase of the electron wave but not the classical path of the electrons. Therefore, the result of the experiment is of entirely quantum-mechanical nature because it originates from variations of the phases or wave surfaces. The change of the phases results from the change of the vector potential, which depends on its boundary values at the coil. These boundary values depend on the current in the coil. The result of

the Moellenstedt's experiment convincingly demonstrates the physical reality of the magnetic vector potential, contrary to the general belief that this quantity is a pure mathematical construct. The invention of the electron-optical biprism and the development of highly coherent field-emission electron guns gave birth to electron holography which has become an important technique for determining electric and magnetic fields in solid objects on an atomic scale [43, 44].

2.3 Ray Properties Associated with the Eikonal

Owing to the existence of the wave or action surfaces, the trajectories of particles originating from a common point can never mingle arbitrarily because the directions of their associated wave vectors remain always perpendicular to the wave surfaces. However, in the presence of an electromagnetic field, the initially *homocentric* bundle of rays will generally not be homocentric elsewhere such that the asymptotes intersect each other in a common point for all wave surfaces. This situation would only be the case for a rotationally symmetric ideal lens, which does not exist for charged particles. As a result, a spherical wave will not remain spherical if it propagates within an electromagnetic field. However, this behavior does not necessarily prevent an ideal imaging. We achieve such a point-to-point imaging if the imaging system transfers an initially outgoing spherical wave from the *object space* in a converging spherical wave in the *image space*. Then, the optical path length $L = S/q_0$ between the object point P_o and the image point P is the same for all rays connecting these *conjugate* points, as depicted in Fig. 2.7. This condition is less stringent since the bundle of rays needs not to be continuously homocentric in the

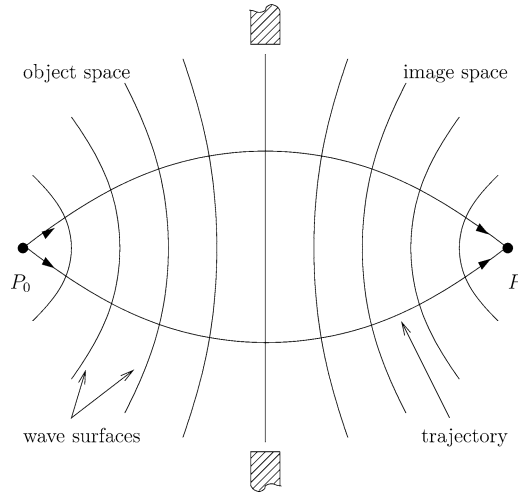


Fig. 2.7. Wave surfaces and particle trajectories in the case of ideal imaging

region between the object and the image. We encounter approximately this situation in an aberration-corrected electron microscope.

The trajectories are perpendicular to the wave surfaces only in the absence of a magnetic field. In this case, the trajectories can never screw around each other. The magnetic field can produce such a twist only because in this case the rays are not orthogonal to the wave surfaces. A measure for the “screwing” of the trajectories is the *circulation*:

$$C = \oint m\vec{v} d\vec{s} = \oint \vec{\nabla} S d\vec{s} + e \oint \vec{A} d\vec{s} = e \iint \vec{B} d\vec{\sigma} = e\Phi_m. \quad (2.62)$$

The line integration has to be taken around a loop enclosing the boundary trajectories of a bundle of rays on a wave surface. We must perform the two-dimensional integration over the area enclosed by the loop. We obtain the last integral by applying *Stokes' theorem* together with $\vec{\nabla} \times \vec{A} = \vec{B}$ and by considering $\oint \vec{\nabla} S d\vec{s} = S - S = 0$. The result demonstrates that the screwing of the trajectories is proportional to the magnetic flux penetrating through the area of the wave surface formed by the loop, which encircles the bundle of rays. In hydrodynamics, the circulation defines the *curl strength* of a flow.

The curvature $\vec{\kappa}$ and torsion τ of the trajectory define the instantaneous change in the course of the particle at any given position. We obtain these quantities most conveniently by considering that the curl of the canonical momentum is zero:

$$\vec{\nabla} \times \vec{p} = \vec{\nabla} \times \vec{\nabla} S = \vec{\nabla} \times m\vec{v} - e\vec{\nabla} \times \vec{A} = \vec{\nabla} \times m\vec{v} - e\vec{B} = 0. \quad (2.63)$$

It should be noted that both $\vec{p} = \vec{p}(\vec{r}, \vec{r}_0)$ and $\vec{v} = \vec{v}(\vec{r}, \vec{r}_0)$ must be conceived as functions of the coordinates of the initial position \vec{r}_0 and the point of observation \vec{r} . This differs from the usual case where one fixes the trajectory by its position and slope at the origin.

The curvature $\vec{\kappa}$ and the torsion τ determine the rotation of the accompanying *Frenet-Serret trihedral* defined by the orthogonal unit vectors \vec{e}_t , $\vec{e}_n = \vec{\kappa}/\kappa$, and $\vec{e}_b = \vec{e}_t \times \vec{e}_n$, as shown in Fig. 2.8. If we know the *tangential unit vector* $\vec{e}_t = \vec{v}/v$ and the electromagnetic field at a given position of the

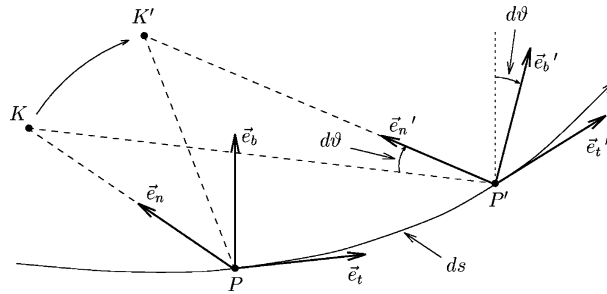


Fig. 2.8. Motion of the accompanying Frenet-Serret trihedral along a curved trajectory in the absence of a tangential component of the magnetic field ($B_t \equiv \vec{e}_t \cdot \vec{B} = 0$)

particle, both the curvature and the torsion of the trajectory can be readily determined from the relations

$$\begin{aligned}\vec{\kappa} &= \kappa \vec{e}_n \frac{d\vec{e}_t}{ds} = (\vec{e}_t \vec{\nabla}) \vec{e}_t = -\vec{e}_t \times (\vec{\nabla} \times \vec{e}_t), \\ \tau &= \frac{d\vartheta}{ds} = -\vec{e}_n \frac{d\vec{e}_b}{ds} = \vec{e}_n \left(\frac{d\vec{e}_n}{ds} \times \vec{e}_t \right) = \frac{\vec{e}_t}{\kappa^2} \left(\vec{\kappa} \times \frac{d\vec{\kappa}}{ds} \right).\end{aligned}\quad (2.64)$$

The tangential vector and the *normal unit vector* \vec{e}_n define the *tangential plane*, which embeds the differential path length. The reciprocal curvature $1/\kappa = \rho$ represents the *radius of curvature* whose origin K defines the *momentary center of curvature* of the trajectory at the point P , as illustrated in Fig. 2.8. The *normal* unit vector \vec{e}_n points toward the center of curvature; the *binormal* unit vector \vec{e}_b is perpendicular to the tangential plane. Both vectors rotate about the tangent by the differential angle $d\vartheta$ if the point P moves along the trajectory by the differential arc length ds .

We obtain the curl of the tangential unit vector from the last equation of (2.63) as

$$\vec{\nabla} \times (mv\vec{e}_t) - e\vec{B} = mv(\vec{\nabla} \times \vec{e}_t) - \vec{e}_t \times \vec{\nabla} mv - e\vec{B} = 0. \quad (2.65)$$

Using this result, we derive from (2.64) the expression

$$\vec{\kappa} = [ev\vec{B} + \vec{v} \times \vec{\nabla} mv] \times \frac{\vec{v}}{mv^3} = \frac{e\vec{B} \times \vec{v}}{mv^2} - \frac{1 + e\varphi/E_0}{2} \frac{\vec{E}_\perp}{\varphi^*} \quad (2.66)$$

for the vector of curvature, where $\vec{E}_\perp = (\vec{e}_t \times \vec{E}) \times \vec{e}_t$ is the component of the electric field strength perpendicular to the direction of the particle velocity. Hence, if both \vec{B} and \vec{E} point in the direction of the velocity, the trajectory will not be curved. This behavior does not hold true for the torsion τ . Employing the relations (2.63) and (2.66), we eventually find from (2.64) after a lengthy calculation for the torsion the expression

$$\tau = \frac{e\vec{v}\vec{B}}{mv^2} - \frac{\vec{\kappa}}{\kappa^2} \left[(\vec{e}_t \vec{\nabla}) \frac{e\vec{B}}{mv} + \vec{e}_t \times (\vec{e}_t \vec{\nabla}) \frac{\vec{\nabla} mv}{mv} \right]. \quad (2.67)$$

The expression in the bracket vanishes for a constant electromagnetic field. In this case, the inverse torsion

$$\frac{1}{\tau} = \rho_L = \frac{mv}{eB_t} \quad (2.68)$$

coincides with the radius ρ_L of the *Larmor rotation*, where $B_t = \vec{B}\vec{e}_t = \vec{B}\vec{v}/v$ is the absolute value of the tangential component of the magnetic field in the direction of the velocity. The corresponding *angle of Larmor rotation* is given by

$$\vartheta_L = \int_{\vec{r}_0}^{\vec{r}} \frac{e\vec{B}}{mv} d\vec{s}. \quad (2.69)$$

It is important to note that the Larmor rotation does not affect the location of the center of curvature. Hence, to guarantee that the normal unit vector \vec{e}_n of the accompanying triad always points in the direction of the center of curvature K , we must rotate the triad back by the angle ϑ_L . Although the torsion results primarily from the tangential component of the magnetic field, as expected from the relation (2.62) for the circulation, this component does not affect the curvature of the trajectory.

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