Successive approximations for charged particle motion

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To H. Rose on the occasion of his 65th birthday

Single particle dynamics in electron microscopes, ion or electron lithographic instruments, particle accelerators, and particle spectrographs is described by weakly nonlinear ordinary differential equations. Therefore, the linear part of the equation of motion is usually solved and the nonlinear effects are then found in successive order by iteration methods.

When synchrotron radiation is not important, the equation can be derived from a Hamiltonian or a Lagrangian. The Hamiltonian nature can lead to simplified computations of particle transport through an optical device when a suitable computational method is used. H. Rose and his school have contributed to these techniques by developing and intensively using the eikonal method. Many ingenious microscopic and lithographic devices were found by Rose and his group due to the simple structure of this method.

The particle optical eikonal method is either derived by propagating the electron wave or by the principle of Maupertuis for time independent fields. Maybe because of the time dependent fields which are often required, in the area of accelerator physics the eikonal method has never become popular, although Lagrange methods had been used sometimes already in early days. In this area classical Hamiltonian dynamics is usually used to compute nonlinear particle motion. Here I will therefore derive the eikonal method from a Hamiltonian quite familiar to the accelerator physics community.

I. INTRODUCTION

The well known Lagrange variational principle requires

$$\delta \int L dt = \delta \int [\dot{\bar{r}} \cdot \dot{q} - \mathcal{H}] dt = 0 \quad (1.1)$$

with the Lagrangian $L$, Hamiltonian $\mathcal{H}$, and generalized momenta $\bar{p}$ and coordinates $\bar{q}$.

In this principle all variations of $\bar{q}(t)$ are allowed and therefore the Euler–Lagrange equations of motion hold,

$$\frac{d}{dt} \partial_{\dot{q}} L(\bar{q}, \dot{\bar{q}}, t) = \partial_{\ddot{q}} L(\bar{q}, \dot{\bar{q}}, t) \quad (1.2)$$

For relativistic single particle motion the Lagrangian is

$$L = -m c \sqrt{\dot{\bar{r}}^2 - \bar{v}^2} + e \bar{r} \cdot \vec{A} - e \Phi \quad (1.3)$$

where the position $\bar{r}(\bar{q})$ is a function of the generalized coordinates $\bar{q}$. The Jacobian matrix $\mathbf{L}$ of this function can be written in the form $\mathbf{L} = (\partial \bar{r} / \partial \bar{q})^T$ and has the elements $\mathbf{L}_{ij} = \partial_{\bar{q}_i} \bar{r}_j$. In this efficient notation $\bar{r}^T$ is the transpose of the $3 \times 1$ matrix $\bar{r}$. The Jacobian matrix of the function $\bar{r}(\bar{q})$ is also $\mathbf{L}$ since $\bar{r} = \sum_{i=1}^{3} \bar{q}_i \partial_{\bar{q}_i} \bar{r} = \mathbf{L} \bar{q}$.

The generalized momentum is $\bar{p} = \partial_{\bar{q}} L = \mathbf{L}^T (m \gamma \dot{\bar{r}} + e \vec{A})$ and the variational principle can thus be written as

$$\delta \int [\bar{p}^T \mathbf{L}^{-1} \dot{\bar{r}} - \mathcal{H}] dt = \delta \int [(m \gamma \dot{\bar{r}} + e \vec{A})^T \mathbf{L} \mathbf{L}^{-1} \dot{\bar{r}} - \mathcal{H}] dt$$

$$= \delta \int [m \gamma \dot{\bar{r}}^2 + e \vec{A}^T \dot{\bar{r}} - \mathcal{H}] dt \quad (1.4)$$

If only variations $\delta_{\mathcal{H}=E}$ are considered which keep the total energy $\mathcal{H} = E$ constant, the variational principle becomes

$$\delta_{\mathcal{H}=E} \int [\bar{p} \cdot \dot{\bar{q}} - \mathcal{H}] dt = \delta_{\mathcal{H}=E} \int \bar{p} \cdot d\bar{q}$$

$$= \delta_{\mathcal{H}=E} \int [m \gamma \dot{\bar{r}}^2 + e \vec{A}^T \dot{\bar{r}}] dt = 0 \quad (1.5)$$

The variational principle for constant total energy is called the principle of Maupertuis. However, in equation (1.4) it does not lead to Euler–Lagrange equations of motion, since not all variations are allowed.

A particle optical device usually has an optical axis or some design curve along which a particle beam should travel. This design curve $\bar{R}(l)$ is parameterized by a variable $l$ and the position of a particle in the vicinity of the design curve has coordinates $x$ and $y$ along the unit vectors $\vec{e}_x$ and $\vec{e}_y$ in a plane perpendicular this curve. This coordinate system is shown in figure 1. The third coordinate vector $\vec{e}_l = d\bar{R}/dl$ is tangential to the design curve and the curvature vector is $\vec{k} = -d\vec{e}_l/dl$.

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The unit vectors $\vec{e}_x$ and $\vec{e}_y$ in the usual Frenet–Serret conoving coordinate system rotate with the torsion of the design curve. If this rotation is wound back, the equations of motion do not contain the torsion of the design curve. The position and the velocity are

\[
\vec{r} = x\vec{e}_x + y\vec{e}_y + \vec{R}(l), \quad \dot{\vec{r}} = \dot{x}\vec{e}_x + \dot{y}\vec{e}_y + h\dot{\vec{e}_l},
\]

with $h = 1 + x\kappa_x + y\kappa_y$. This method is described in \cite{3} and \cite{10} and is mentioned here since design curves with torsion are becoming important when considering particle motion in helical wigglers, undulators, and wavelength shifters \cite{11}, and for polarized particle motion in helical dipole Siberian Snakes \cite{12}.

Since all variations are allowed, the integrand is a very simple new Lagrangian

\[
\tilde{L} = m\gamma v \sqrt{x'^2 + y'^2 + h^2 + e(x' A_x + y' A_y + h A_l)}
\]

which leads to Euler–Lagrange equations of motion

\[
\begin{align*}
\dot{\tilde{p}}_x &= \partial_x\tilde{L}, & \dot{\tilde{p}}_y &= \partial_y\tilde{L}, \\
\dot{\tilde{p}}_l &= \partial_l\tilde{L}.
\end{align*}
\]

The integral $\int_{l_0}^l \tilde{L}(l) dl$ is called the eikonal.

Since the Hamiltonian formulation is very common in the area of accelerator physics, we will show how the eikonal can be derived from a Hamiltonian formulation.

The equations of motion for the three generalized coordinates $x(t)$, $y(t)$, and $l(t)$ can be obtained from the Hamiltonian

\[
\mathcal{H} = e\Phi + \sqrt{m^2c^2 + (\tilde{p}_x - eA_x)^2 + (\tilde{p}_y - eA_y)^2 + (\tilde{p}_l/h - eA_l)^2}.
\]

In the case of time independent fields, $\mathcal{H}$ is the conserved total energy $E$ and there are only five independent variables, rather than six. Note that the velocity dependent or non holonomic \cite{13} boundary condition $\mathcal{H}(\tilde{p}, \tilde{q}, \dot{\tilde{q}}, t) = E$ cannot be included in the Lagrange formalism directly. But in the Hamilton formalism this can be done. Furthermore, a switch of independent variable from $t$ to $l$ can easily be done in the Hamiltonian formulation. The Lagrange formulation is therefore abandoned (too easily, as will be shown later). In the variational condition

\[
\delta \int [x\tilde{p}_x + y\tilde{p}_y + l\tilde{p}_l - \mathcal{H}] dt = 0
\]

one can change to the independent variable $l$ as follows:

\[
\delta \int [x'\tilde{p}_x + y'\tilde{p}_y + (-t')\mathcal{H} - (-\tilde{p}_l)] dl = 0.
\]

The six canonical coordinates are now $x$, $\tilde{p}_x$, $y$, $\tilde{p}_y$, $-t$, and $\mathcal{H}$, and the new Hamiltonian is given by $\mathcal{H} = -\tilde{p}_l$ which has to be expressed as a function of the six coordinates \cite{14,15}.

\[
\dot{H} = -h \left[ eA_l + \sqrt{\left(\mathcal{H} - e\Phi\right)^2 - (\tilde{p}_x - eA_x)^2 - (\tilde{p}_y - eA_y)^2} \right].
\]

In the Hamilton formalism it is simple to take advantage of the fact that the total energy is conserved for time independent fields; $\mathcal{H}' = \partial_t \mathcal{H} = 0$ leads to $\mathcal{H} = E$. Then from the six coordinates only the first four have to be considered, leading to the Lagrangian

\[
\tilde{L} = x'\tilde{p}_x + y'\tilde{p}_y - \tilde{H}.
\]
From \( x' = \partial_{\tilde x} \tilde H = \frac{\text{d}}{\text{d}t}(\tilde p_x - eA_x) \), \( y' = \partial_{\tilde p_y} \tilde H = \frac{\text{d}}{\text{d}t}(\tilde p_y - eA_y) \) where \( \sqrt{\cdot} \) is the square root in \( \tilde H \) one obtains
\[
\sqrt{\cdot} = \frac{h}{\sqrt{(E - e\Phi)^2 - (mc^2)^2}} \frac{1}{x'^2 + y'^2 + h^2}, \\
\tilde p_x = \frac{\sqrt{\cdot} x' + eA_x}, \quad \tilde p_y = \frac{\sqrt{\cdot} y' + eA_y}, \\
\tilde L = m\gamma v \sqrt{x'^2 + y'^2 + h^2 + e(x' A_x + y' A_y + h A_l)}.
\] (1.18)

for \( m\gamma v = \sqrt{(E - e\Phi)^2/c^2 - (mc^2)^2} \). The very simple Lagrangian \( \tilde L \) agrees with the integrand (1.8) of the eikonal.

In the following it will be shown how the Hamiltonian and the Lagrangian equations of motion for the particle trajectory \( \tilde q(l) \) can be solved in an iterative way. We write a general equation of motion for a coordinate vector \( \tilde z \) in the form
\[
\tilde z' = f^1(\tilde z, l) + f^{2,2}(\tilde z, l)
\] (1.19)
where we assume that \( \tilde z = 0 \) is a solution of the differential equation. Furthermore, we assume \( \tilde z \) to be small and let \( f^1 \) be linear in the coordinates. We assume that the nonlinear part of the equation of motion can be expanded in a Taylor series \( f^{2,2} \). The linearized equation of motion is solved by a trajectory \( \tilde z_1(l) = M(l) \tilde z \), which depends linearly on the initial coordinates. For the transport matrix \( M(l) \) we therefore have
\[
M'l \tilde z_1 = f^1 M' \tilde z
\] (1.20)
for all coordinate vectors \( \tilde z_1; f^1 \) being the Jacobian matrix of \( f^1 \).

One can write every solution of (1.19) as \( \tilde z(l) = M(l) \tilde z(0) \), leading to the equation of motion for \( \tilde z \).
\[
M' \tilde z + M \tilde z' = f^1 M \tilde z + f^{2,2} \tilde z
\] (1.21)
The Taylor coefficients of \( \tilde z(l) \) with respect to the initial coordinates \( \tilde z_1 = \tilde z(0) \) are called aberration coefficients. With equation (1.20) one obtains
\[
\tilde z(l) = M(l) \{ \tilde z_1 + \int_0^l M^{-1}(\tilde l) f^{2,2}(\tilde z(l)) \} \text{d} \tilde l.
\] (1.22)

Now we assume that the general solution \( \tilde z(\tilde z_1, l) \) can be expanded in a power series with respect to the initial coordinates. Then symbolizing the \( j \)th order Taylor polynomial with \([\cdot; j]\), we write the orders up to \( j \) as \( \tilde z_j = [\tilde z(\tilde z_1, l)]_j \), i.e. we use lower indices to describe the order of \( \tilde z_j \). The upper index in \( f^j \) describes the order in \( \tilde z \), which is in turn a nonlinear function of \( \tilde z_1 \). When \( \tilde z_{n-1} \) is known, one can iterate the expansion up to order \( n \) with equation (1.22), since
\[
\tilde z_n = M(l) \{ \tilde z_1 + \int_0^l M^{-1}(\tilde l) f^{2,2}([\tilde z_l-1]; n) \} \text{d} \tilde l.
\] (1.23)

The zeroth order of the expansion with respect to the coordinates must vanish, which means that the trajectory \( \tilde q = 0 \) must satisfy the equation of motion for some momentum \( p(0) \). Additionally we require that the vector potential on the design curve is gauged to zero. This can always be achieved. The canonical momentum \( p \) then also vanishes for the trajectory \( \tilde q = 0 \). It then follows that the Hamiltonian and the Lagrangian have no components linear in the coordinates and momenta. When computing trajectories through a particle optical device, it is customary to normalize the momenta to the initial design momentum \( p_0 = p(0) \). The following two dimensional generalized coordinates are therefore used:
\[
\tilde q = \begin{pmatrix} x \\ y \end{pmatrix}, \quad \tilde p = \begin{pmatrix} \tilde p_x/p_0 \\ \tilde p_y/p_0 \end{pmatrix},
\] (1.24)
\[
L(\tilde q, \tilde q', l) = \tilde L/p_0, \quad \tilde p = \partial_{\tilde q} L, \quad \tilde p' = \partial_{\tilde q'} L, \quad H(\tilde q, \tilde p, l) = \tilde H/p_0, \quad \tilde q' = \partial_{\tilde p} H, \quad \tilde p' = -\partial_{\tilde q} H.
\]
The Euler–Lagrange equations lead to the second order differential equations \( \frac{\text{d}}{\text{d}l} \partial_{\tilde q} L = \partial_{\tilde q} H \) for the two dimensional vector \( \tilde q \).

II. SUCCESSIVE APPROXIMATION IN TERMS OF HAMILTONIANS

In the Hamilton formalism one obtains first order equations of motion for the four dimensional vector \( \tilde z^T = (q_1, q_2, p_1, p_2) \). With the antisymmetric matrix \( J \) one can write the equation of motion as
\[
J \tilde z' = \begin{pmatrix} 0 & 1_2 \\ -1_2 & 0_2 \end{pmatrix},
\] (2.1)
with the \( 2 \times 2 \) identity and zero matrices \( 1_2 \) and \( 0_2 \). This structure implies special symmetries for the transport maps \( \tilde M \) of particle optics. These maps describe how the final phase space coordinates \( \tilde z_f = \tilde M(\tilde z) \) of a particle, after flying through an optical device, are related to the initial coordinates \( \tilde z \). These maps are often weakly nonlinear and can be expanded in a Taylor expansion. The Hamiltonian nature implies that the Jacobian \( \tilde M = (\partial_{\tilde z} \tilde M^T)^T \) of any transport map \( \tilde M(\tilde z) \) is symplectic \( [13] \), meaning that
\[
\tilde M J \tilde M^T = J.
\] (2.2)

For the successive approximations we separate the equation of motion into its linear and nonlinear part,
\[
\tilde z' = J \partial_{\tilde z}(H^2 + H^{\geq 3}).
\] (2.3)
After we have solved for the linear transport matrix \( \vec{Z}_n \), we can iterate by equation (1.23) which takes the form

\[
\vec{z}_n = \mathbf{M}\{\vec{z}_n + \int_0^l \mathbf{M}^{-1} \mathbf{J} \partial_\vec{z} \mathbf{H}^{\geq 3}(\vec{z}_{n-1})_n d\vec{t}\} \quad (2.4)
\]

With the relation \( \mathbf{M}^{-1} \mathbf{L} = \mathbf{J} \mathbf{M}^T \) from equation (2.3) this can be written as

\[
\vec{z}_n = \mathbf{M}\{\vec{z}_n + \int_0^l \mathbf{M}^T [\partial_\vec{z} \mathbf{H}^{\geq 3}(\vec{z}_{n-1})_n] d\vec{t}\} \quad (2.5)
\]

The corresponding equation for the aberrations \( \vec{\zeta}_n = \mathbf{M}^{-1} \vec{z}_n \) becomes

\[
\vec{\zeta}_n = \vec{z}_n + \int_0^l \partial_\vec{z} \mathbf{H}^{\geq 3}(\mathbf{M} \vec{z}_{n-1})_n d\vec{t} \quad (2.6)
\]

This form of the iteration equation is quite simple. However, since the Hamiltonian \( \mathbf{H} \) is a complicated function, the evaluation of the four integrals can become very cumbersome.

### III. SUCCESSIVE APPROXIMATION IN TERMS OF LAGRANGIANS

In\(^{(3)}\) Rose used a variational principle to derive a successive approximation to nonlinear motion based on the eikonal. This method iterates position \( \vec{q} \) and momentum \( \vec{p} \) in their nonlinear dependence on the initial position \( \vec{q}_0 \) and momentum \( \vec{p}_0 \). Knowing the order \( n-1 \) dependence \( \vec{q}_n-1 \) and \( \vec{p}_n-1 \), one has to compute \( \vec{q}_n \) by differentiation of \( \vec{q}_n \) or by inversion of \( \vec{p} = \partial_\vec{q} L(\vec{q}, \vec{q}', \vec{t}) \). Then the eikonal can be evaluated by computing the order \( n \) dependence \( \vec{q}_n \) and \( \vec{p}_n \). In general it can be cumbersome to compute \( \vec{q}_n \) and therefore here we derive a new version of the eikonal method, which iterates directly \( \vec{q}_n \) rather than the momentum.

In deriving the simple form of equation (2.2), advantage has only been taken of the symplectic first order transfer matrix. We therefore wish to exploit this advantage again by working with new coordinates which are identical with the canonical \( \vec{q} \) and \( \vec{p} \) up to first order so that the new coordinates lead to the same first order transport matrix \( \mathbf{M} \). To first order one obtains

\[
\vec{p} = \partial_\vec{q} L = \frac{p(s)}{p_0} \vec{q}' + \frac{e}{p_0} (A'_1) + \mathcal{O}^2(\vec{q}', \vec{q}'') \quad (3.1)
\]

where \( p(s) \) is the momentum of a particle traveling on the design curve \( \vec{q} = 0 \), and the upper index 1 specifies the part of the vector potential linear in \( x \) and \( y \). We therefore work with the coordinates

\[
\vec{\tilde{q}} = \left( \begin{array}{c} \vec{q} \\ \vec{u} \end{array} \right) = \left( \begin{array}{c} \frac{p(s)}{p_0} \vec{q}' + \frac{e}{p_0} (A'_1) \\ \vec{u} \end{array} \right) \quad (3.2)
\]

Moreover, it can be shown\(^{(16,17,18)}\) that the contribution from the vector potential can be gauged to vanish whenever there is no longitudinal magnetic field \( B_0 \partial_\vec{z} \) on the design curve. Then if one investigates trajectories which start with momentum \( \vec{p}_0 \) in a region free of such a field, we have the simple relation \( \vec{u}_n = \vec{q}_n' \).

By splitting the Lagrangian into its second order and its higher order part, the equation of motion becomes

\[
\vec{\tilde{Q}}' = \left( \begin{array}{c} \vec{q}' \\ \vec{u}' \end{array} \right) = \left( \frac{p(s)}{p_0} \vec{q}' - \frac{e}{p_0} (A'_1) \right) - \left( \frac{d}{dt} \partial_\vec{q} L^{\geq 3} - \partial_\vec{q} L^{\geq 3} \right) \quad (3.3)
\]

After having solved the linearized equation of motion, we obtain with equation (1.23)

\[
\vec{\tilde{Q}} = \mathbf{M}\{\vec{Q}_1 - \int_0^l \mathbf{M}^{-1} \left( \frac{d}{dt} \partial_\vec{q} L^{\geq 3} - \partial_\vec{q} L^{\geq 3} \right) d\vec{t}\} \quad (3.4)
\]

\[
\vec{\tilde{Q}} = \mathbf{M}\{\vec{Q}_1 + \int_0^l \mathbf{M}^T \left( \frac{d}{dt} \partial_\vec{q} L^{\geq 3} - \partial_\vec{q} L^{\geq 3} \right) d\vec{t}\} \quad (3.5)
\]

An integration by parts leads to

\[
\vec{\tilde{Q}} = \mathbf{M}\{\vec{Q}_1 - \int_0^l \mathbf{M}^{-1} \left[ \partial_\vec{q} \vec{Q}_1 \partial_\vec{q} L^{\geq 3} = \partial_\vec{q} \vec{Q}_1 \partial_\vec{q} L^{\geq 3} \right] \quad (3.6)
\]

Note that the \( A'_1 \), \( A'_1 \), \( p(s) \) and \( p_0 \) of equation (3.2) drop out of the right hand side of equation (3.6) owing to the multiplications by the zeros in equation (3.5). The second order \( L^2 \) of the Lagrangian is a quadratic form in which
every quadratic combination of the \( \vec{q} \) and \( \vec{q}' \) can occur. It can be written using a matrix \( L^2 \) as \( L^2 = \vec{Q}^T L^2 \vec{Q} \). Part of the above integrand can be rewritten as
\[
q_{22}^T \partial_q^T \vec{L}^2 + \vec{q}_{22}^T \partial_q L^2 = \vec{Q}_{22}^T L^2 \vec{Q} + \vec{Q}^T L^2 \vec{Q}_{22} .
\] (3.7)
For convenience we write \( L^2(\vec{u}) = \vec{d}^T L^2 \vec{d} \). Another integration by parts in equation (3.6) leads to
\[
M^{-1} \dot{\vec{Q}} = \dot{\vec{Q}}_i - J \int_0^t \left[ \partial_{\vec{Q}_i} (L \vec{q}^3 + L^2(\vec{Q}_{22})) + (\partial_{\vec{Q}_i} q_{22}^T) \partial_q L^2 (\vec{Q}_1) + (\partial_{\vec{Q}_i} q_{22}^T) \partial_q L^2 (\vec{Q}_{22}) \right] d\vec{d} + J \left[ (\partial_{\vec{Q}_i} q_{22}^T) \partial_q L + (\partial_{\vec{Q}_i} q_{22}^T) \partial_q L^3 \right]_0^t .
\] (3.8)
The first part of the integral contains \( L_E = L \vec{q}^3 + L^2(\vec{Q}_{22}) \). The integral \( J \int_0^t L_E d\vec{d} \) is called the perturbation eikonal. This scheme embodies the essential requirement that the \( n+1 \) order dependence of \( L_E \) on the initial variables \( \vec{Q}_i \) can be computed already when \( Q_{n-1} \) is known; \( \vec{Q}_n \), does not need to be known. For an iteration of \( \vec{Q}_n \), knowledge of \( \vec{Q}_{n-1} \) is sufficient. Since \( \vec{q}_i \) satisfies the first order equation of motion, we can use the relation
\[
\partial_{\vec{Q}_i} L^2 (\vec{Q}_1) = \frac{d}{dt} \partial_{\vec{Q}_i} L^2 (\vec{Q}_1)
\] to perform another integration by parts,
\[
M^{-1} \dot{\vec{Q}} = \dot{\vec{Q}}_i - J \int_0^t L_E d\vec{d} + \int \left[ \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L + \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L^3 \right] d\vec{d} + \int \left[ \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L + \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L^3 \right]_0^t .
\] (3.9)
The first part of the integral contains \( L_E = L \vec{q}^3 + L^2(\vec{Q}_{22}) \). The integral \( J \int_0^t L_E d\vec{d} \) is called the perturbation eikonal. This scheme embodies the essential requirement that the \( n+1 \) order dependence of \( L_E \) on the initial variables \( \vec{Q}_i \) can be computed already when \( Q_{n-1} \) is known; \( \vec{Q}_n \), does not need to be known. For an iteration of \( \vec{Q}_n \), knowledge of \( \vec{Q}_{n-1} \) is sufficient. Since \( \vec{q}_i \) satisfies the first order equation of motion, we can use the relation
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\] to perform another integration by parts,
\[
M^{-1} \dot{\vec{Q}} = \dot{\vec{Q}}_i - J \int_0^t L_E d\vec{d} + \int \left[ \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L + \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L^3 \right] d\vec{d} + \int \left[ \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L + \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L^3 \right]_0^t .
\] (3.9)
\( \partial_{\vec{Q}_i} L_E \) is the part of \( \partial_{\vec{Q}_i} L \) which up to order \( n \) in \( \vec{Q}_i \) does not depend on \( \vec{Q}_n \). Similarly the term inside the integral is simply the part of \( \partial_{\vec{Q}_i} q_{22}^T \partial_q L \) which up to order \( n \) does not depend on \( \vec{Q}_n \). Therefore write
\[
\partial_{\vec{Q}_i} q_{22}^T \partial_q L - \partial_{\vec{Q}_i} q_{22}^T \partial_q L^2 - \partial_{\vec{Q}_i} q_{22}^T \partial_q L^3 = \{(\partial_{\vec{Q}_i} q_{22}^T) \partial_q L_E \} .
\]
If we now express the Lagrangian in terms of the aberrations \( \vec{\xi} \) with \( \vec{Q} = M \vec{\xi} \), we obtain the iteration equation
\[
\vec{\xi}_n - \vec{\xi}_n = \vec{\xi}_n - \vec{Q}_i - J \int_0^t L_E (M \vec{\xi}_{n-1}) d\vec{d} + \int \left[ \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L_E \right] d\vec{d} + \int \left[ \left( \partial_{\vec{Q}_i} q_{22}^T \right) \partial_q L_E \right]_0^t .
\] (3.10)
When computing \( \vec{\xi}_n \) from \( \vec{\xi}_{n-1} \) with this iteration equation, all parts of the right hand side which contribute to higher orders are neglected, as indicated by \( =n \). This iteration equation can have several advantages over the Hamiltonian iteration equation (1.23):

\[a\] The Lagrangian (1.3) is a much simpler function than the Hamiltonian (1.14).

\[b\] The derivative in equation (3.10) is performed after the integral has been evaluated. Therefore only one integral has to be computed and it describes all four coordinates of \( \vec{\xi}_n \).

\[c\] The fact that the various coordinates are the derivatives with respect to initial conditions yields very simple relations between the various expansion coefficients of \( \vec{\xi}_n \), which are the so called aberration coefficients of particle optical devices. These relations can be much simpler than relations entailed by the symplectic symmetry implicit in the Hamiltonian formulation.

\[d\] The second pair of coordinates in equation (3.2) can be calculated very easily. With equations (1.21) and (1.23), the equation of motion for \( \vec{\xi} \) is
\[
M \ddot{\vec{\xi}} = \left( \begin{array}{ccc} 0 \\ \frac{2}{c^2} \partial_q L^3 - \partial_q L^3 \end{array} \right) .
\] (3.11)

After having computed \( \vec{q}_n = M_{2 \times 4} \vec{\xi}_n \) by iteration, the derivative \( \vec{q}' \) can then easily be computed as \( \vec{q}'_n = M_{2 \times 4} \vec{\xi}_n \) using equation (3.11). One thus only needs to iterate the two dimensional vector \( \vec{q}_n \) and not a four dimensional vector \( \vec{\xi}_n \) as in the Hamiltonian iteration procedure.

**IV. SUCCESSIVE APPROXIMATION FOR SPIN ORBIT MOTION**

The time variation of a spin \( \vec{s} \) in the rest frame of a particle is described by the so called Thomas–BMT equation \( \vec{\xi} = \vec{\Omega}_{BMT} \times \vec{s} \) [21] where
\[
\vec{\Omega}_{BMT} = -\frac{q}{m c} \left((a \gamma + 1) \vec{B}_2 + (1 + a) \vec{B}_1 \right) \left( -\frac{2}{c^2} \vec{E}(a + \frac{1}{1 + \gamma}) \right)
\] (4.1)
with the electric field \( \vec{E} \), the parts of the magnetic field \( \vec{B} \) which are perpendicular (\( \perp \)) and parallel (\( \parallel \)) to the particle’s velocity, and the anomalous gyro-magnetic factor \( a = \frac{e}{2 m} \).

Changing to the comoving coordinate system of figure [1], we obtain \( \vec{s} = S_x e_x + S_y e_y + S_z e_z \) and \( \vec{s}' = (S'_x - S_x \kappa_x) e_x + (S'_y - S_y \kappa_y) e_y + (S'_z + S_z \kappa_x + S_x \kappa_y) e_z \). The equation of motion for the vector \( \vec{S} \) of these spin components is then
\[
\vec{S}' = \vec{\Omega} \times \vec{S} ,
\] (4.2)
\[
\vec{\Omega} = \vec{\Omega}_{BMT} \frac{\hbar}{v} \sqrt{x^2 + y^2 + z^2} - \vec{K} \times \vec{e}_l .
\]
The equations of motion for the phase space vector $\tilde{z}$ and the spin $\tilde{S}$ have the form

$$\tilde{z}' = \tilde{f}(\tilde{z}, l), \quad \tilde{S}' = \tilde{\Omega}(\tilde{z}, l) \times \tilde{S}. \quad (4.3)$$

The general solutions transporting the coordinates along the optical system, starting at the initial values $\tilde{z}_i, \tilde{S}_i$, is given by the transport map $\mathcal{M}$ and the rotation matrix $R \in SO(3)$,

$$\tilde{z}(l) = \mathcal{M}(\tilde{z}_i, l), \quad \tilde{S}(l) = R(\tilde{z}_i, l) \tilde{S}_i. \quad (4.4)$$

In order to find the general solution, one could compute the nine coefficients of the rotation matrix by solving the differential equation

$$R_{ij}(\tilde{z}_i, l)' = \epsilon_{ijk} M_k R_{kj}(\tilde{z}_i, l), \quad (4.5)$$

where the vector product was expressed by the totally antisymmetric tensor $\epsilon_{ijk}$. However, computing the nine components of the rotation matrix seems inefficient, since a rotation can be represented by three angles. It has turned out to be most efficient to represent the rotation of spins by the quaternion $A$ which gives the rotation transformation in the SU(2) representation as

$$A = a_0 \mathbf{1} - i \vec{a} \cdot \vec{\sigma}. \quad (4.6)$$

Here $\mathbf{1}$ is the $2 \times 2$ identity matrix and the elements of the vector $\vec{\sigma}$ are the three dimensional Pauli matrices. When a rotation by an angle $\phi$ is performed around the unit vector $\vec{e}$, the quaternion representation of the rotation has $a_0 = \cos(\phi/2)$ and $\vec{a} = \sin(\phi/2)\vec{e}$. Therefore $a_0^2 + \vec{a}^2 = 1$ and the identity transformation is represented by $a_0 = 1$.

If a particle traverses an optical element which rotates the spin according to the quaternion $A$ and then passes through an element which rotates the spin according to the quaternion $B$, the total rotation of the spin is given by

$$C = c_0 \mathbf{1} - i \vec{c} \cdot \vec{\sigma} = (b_0 \mathbf{1} - i \vec{b} \cdot \vec{\sigma})(a_0 \mathbf{1} - i \vec{a} \cdot \vec{\sigma})$$

$$= (b_0a_0 - \vec{b} \cdot \vec{a}) \mathbf{1} - i(b_0\vec{a} + \vec{b}a_0 + \vec{b} \times \vec{a}) \cdot \vec{\sigma}. \quad (4.7)$$

The concatenation of quaternions can be written in matrix form as

$$\tilde{C} = \begin{pmatrix} c_0 \\ \vec{c} \end{pmatrix} = \tilde{B} \begin{pmatrix} a_0 \\ \vec{a} \end{pmatrix}, \quad (4.8)$$

$$\tilde{B} = \begin{pmatrix} b_0 & -b_1 & -b_2 & -b_3 \\ b_1 & b_0 & -b_3 & b_2 \\ b_2 & b_3 & b_0 & -b_1 \\ b_3 & -b_2 & b_1 & b_0 \end{pmatrix}. \quad (4.9)$$

This concatenation of two quaternions can be used to find a differential equation for the spin rotation.

While propagating along the design curve by a distance $dl$, spins are rotated by an angle $\Omega dl = \Omega/zdl$ around the vector $\Omega$. After having been propagated to $l$ by the quaternion $A$, a spin gets propagated from $l$ to $l + dl$ by the quaternion with $b_0 = 1$ and $\vec{b} = \frac{1}{2} \Omega dl$. The resulting total rotation is given by $A + A'dl$ and we obtain the differential equation

$$\begin{pmatrix} a_0' \\ \vec{a}' \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & -\Omega_1 & -\Omega_2 & -\Omega_3 \\ \Omega_1 & 0 & -\Omega_3 & -\Omega_2 \\ -\Omega_2 & \Omega_3 & 0 & -\Omega_1 \\ -\Omega_3 & -\Omega_2 & \Omega_1 & 0 \end{pmatrix} \begin{pmatrix} a_0 \\ \vec{a} \end{pmatrix}. \quad (4.10)$$

Writing the matrix as $\Omega$ and the vector as $\vec{A}$, the spin orbit equation of motion has the form

$$\tilde{z}' = \tilde{f}(\tilde{z}, l), \quad \vec{A} = \Omega(\tilde{z}, l) \vec{A}. \quad (4.11)$$

The starting conditions are $\tilde{z}(0) = \tilde{z}_0, a_0 = 1$, and $\vec{a} = 0$. The quaternion $\vec{A}$ depends on the initial phase space coordinates $\tilde{z}_i$ and can be expanded in a Taylor series with respect to these coordinates. In the following we want to devise an iteration method for $\vec{A}_n$, which is the Taylor expansion to order $n$ of $\vec{A}$.

The rotation vector $\vec{\Omega}$ is split into its value on the design curve and its phase space dependent part as $\vec{\Omega}(\tilde{z}, l) = \tilde{\Omega}(\tilde{z}, l) + \Omega^2(\tilde{z}, l)$. The spin motion on the design curve is given by $\vec{A}_0(l) = \tilde{\Omega}(\tilde{z}, l) \vec{A}_0$. Similarly to equation (4.12), spin aberrations are defined with respect to the leading order motion. Small phase space coordinates will create a rotation which differs little from $\vec{A}_0$ and the $\tilde{z}$ dependent rotation $\Omega \vec{A}_0(l)$ and we write the phase space dependent rotation as a concatenation of $\vec{A}_0$ and the $\tilde{z}$ dependent rotation $\Omega \vec{a}$ which reduces to the identity for $\tilde{z} = 0$ by requiring that the aberrations $\delta$ and $\tilde{\delta}$ vanish on the design curve. With equation (4.14) we obtain

$$\vec{A} = \vec{A}_0 \left( \begin{array}{c} 1 + \delta \\ \tilde{\delta} \end{array} \right). \quad (4.15)$$

The quaternion $\vec{A}$ is now inserted in the differential equation (4.10) to obtain

$$\vec{A}_0 \left( \begin{array}{c} 1 + \delta \\ \tilde{\delta} \end{array} \right) + \vec{A}_0 \left( \begin{array}{c} \delta' \\ \tilde{\delta}' \end{array} \right) = (\tilde{\Omega}_0 + \tilde{\Omega}_1) \vec{A}_0 \left( \begin{array}{c} 1 + \delta \\ \tilde{\delta} \end{array} \right). \quad (4.16)$$

Taking into account the equation on the design curve and the fact that $\vec{A}_0^T$ describes the inverse rotation of $\vec{A}_0$, we obtain

$$\left( \begin{array}{c} \delta' \\ \tilde{\delta} \end{array} \right) = \left( \begin{array}{c} \tilde{\Omega}^T_1 \tilde{A}_0 \\ \tilde{\Omega} \end{array} \right) \left( \begin{array}{c} 1 + \delta \\ \tilde{\delta} \end{array} \right) = \tilde{\Omega}(\tilde{z}, l) \left( \begin{array}{c} 1 + \delta \\ \tilde{\delta} \end{array} \right). \quad (4.17)$$

Writing the Taylor expansion to order $n$ in $\tilde{z}_i$ one finally obtains the iteration equation

$$\left( \begin{array}{c} \delta_n \\ \tilde{\delta}_n \end{array} \right) = n \int_0^l \tilde{\Omega}(\tilde{z}_n) \left( \begin{array}{c} 1 + \delta_{n-1} \\ \tilde{\delta}_{n-1} \end{array} \right) dl, \quad \left( \begin{array}{c} \delta_0 \\ \tilde{\delta}_0 \end{array} \right) = 0. \quad (4.18)$$
This iteration method was used for the spin transport in the program SPRINT [22] and was evaluated using MATHEMATICA in [23].

In the case of successive approximation in terms of the Hamiltonian, the various aberration coefficients were related by the symplectic symmetry. With the Lagrange formalism the various aberration coefficients were related by their being derivatives of a common integral with respect to different initial coordinates. In the case of the successive approximation for spin motion, the various aberration coefficients in \( \delta \) and \( \delta \) are related by the relation

\[
(1 + \delta)^2 + \delta^2 = 0.
\]

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