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Gauge Invariance in the Eikonal Method

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The eikonal method of charged particle optics requires a multipole expansion of the magnetic vector potential. A procedure is outlined which allows a direct computation of the vector potential from the multipole expansion of the magnetic scalar potential. It is shown how the vector potential and the eikonal adopt a simple form by choosing a suitable gauge.

1 Introduction

In electron microscopy and accelerator physics the motion of particles near a reference curve is of interest. To describe the properties of such a particle optical device, the coordinates $\vec{z}_f$ in the end plane of the device have to be expressed as a function of the initial coordinates $\vec{z}_i$:

$$\vec{z}_f = \mathcal{M}(\vec{z}_i) \ . \tag{1}$$

The components of $\vec{z}$ are the space coordinates $\vec{r}$ and the vector components of the canonical momentum $\vec{p}$. It is useful to expand this function or map $\mathcal{M}$ in a Taylor series about a central curve. This can be done by evaluating the equation of motion in Taylor expansions [1] or more effectively by using the eikonal method which yields simpler formulas and automatically satisfies the symplectic condition [2].

It is advantageous to describe the electric and the magnetic field by scalar potentials and to expand the potentials in plane multipoles about the reference curve [3] because the multipole coefficients are experimentally accessible. The magnetic vector potential $\vec{A}$ is needed for calculating the eikonal

$$S = \int_{\text{path}} \vec{p} d\vec{s} = \int_{\text{path}} (m\vec{v} + q\vec{A}) d\vec{s} \tag{2}$$

where $d\vec{s}$ is an element of the path taken by a particle with kinematic momentum $m\vec{v}$ and charge q. In the traditional way the computation of the vector potential is one of the most cumbersome parts of deriving expansion coefficients of $\mathcal{M}$ by the eikonal method.

Recently it has been pointed out [2] that the procedure to compute the vector potential from the scalar potential can be simplified considerably by choosing a suitable gauge function. A mistake mentioned in [4] will be corrected and the method will be explained in detail.

2 Curvilinear coordinates and complex notation

The coordinates near the central curve of reference will be written in complex notation. A space point near this reference curve is described by a vector with three components. Let z be the path length of this curve. Then all space points which lie on a plane perpendicular to the reference curve have the same z-component. In this plane we introduce a rectangular cartesian x, y coordinate system. The x-axis is located in the horizontal plane as depicted in Fig.1a. For mathematical simplicity it is advantageous to describe the off-axial position by the complex coordinates

$$w = x + iy \quad , \qquad \bar{w} = x - iy \; . \tag{3}$$

The metric coefficients of the curvilinear coordinate system shown in Fig.1b are

Place for Fig.1

$$g_1 = |\frac{d\vec{r}}{dx}| = 1 \quad , \qquad g_2 = |\frac{d\vec{r}}{dy}| = 1 \quad , \qquad g_3 = |\frac{d\vec{r}}{dz}| = |\frac{\rho^2 - \vec{r}\vec{\rho}}{\rho^2}| \tag{4}$$

where ρ is the local radius of curvature of the reference curve. The last relation is simplified by using the complex curvature

$$\Gamma = \frac{\rho_x + i\rho_y}{\rho^2} \quad , \qquad g_3 = h = 1 - \Re\{\bar{w}\Gamma\} \; . \tag{5}$$

The partial derivatives ∂_x, ∂_y with respect to the coordinates x and y are related to the partial derivatives with respect to the complex coordinates w and $\bar{w}$ via the formulas

$$\begin{aligned} \partial_x &= 2\Re\{\partial_w\} \quad , & \partial_y &= -2\Im\{\partial_w\} \; , \\ \partial_w &= \frac{1}{2}(\partial_x - i\partial_y) \quad , & \partial_{\bar{w}} &= \frac{1}{2}(\partial_x + i\partial_y) \end{aligned} \tag{6}$$

where $\Re\{\ldots\}$ and $\Im\{\ldots\}$ denote the real and imaginary part, respectively.

3 The magnetic scalar potential

In the case of static fields the magnetic field $\vec{B}(\vec{r})$, at a point $\vec{r}$ without electrical current, can be derived from a magnetic scalar potential $\psi(\vec{r})$:

$$\vec{B}(\vec{r}) = -\nabla\psi(\vec{r}) \tag{7}$$

where $\psi(\vec{r})$ satisfies the Laplace equation

$$\nabla^2\psi(\vec{r}) = 0. \tag{8}$$

By employing the complex notation introduced in section 2 the Laplace equation in the curvilinear coordinate system adopts the form

$$\nabla^2\psi = \frac{1}{h}\{2\partial_w(h\partial_{\bar{w}}\psi) + 2\partial_{\bar{w}}(h\partial_w\psi) + \partial_z(\frac{1}{h}\partial_z\psi)\} = 0\ . \tag{9}$$

The solution can be expanded in a power series about an arbitrary curve. The expansion coefficients [5, 3, 6] have an intuitive meaning. A field of symmetry C_ζ about the reference curve which does not vary with the path length z has the potential $\psi = \Re\{\Psi_\zeta \bar{w}^\zeta\}$ because this harmonic polynomial satisfies the Laplace equation and the required symmetry. The multipole coefficient Ψ_ζ of symmetry C_ζ is generally complex. Its phase describes the orientation of the multipole with respect to the x, y coordinate system. Therefore rotational symmetric fields are described by the real multipole coefficient Ψ_0. If the field varies with path length z, a power series expansion

$$\psi(\vec{r}) = \Re\{\sum_\zeta^\infty \sum_\lambda^\infty a_{\zeta\lambda}(z)(w\bar{w})^\lambda \bar{w}^\zeta\} \tag{10}$$

exists where the multipole coefficients

$$a_{\zeta 0}(z) = \Psi_\zeta(z) \tag{11}$$

are functions of the z-coordinate. In the case of a straight reference curve the Laplace equation yields

$$4\lambda(\lambda+\zeta)a_{\zeta\lambda} + \partial_z^2 a_{\zeta\lambda-1} = 0\ , \tag{12}$$

$$a_{\zeta\lambda} = (-1)^\lambda \frac{\zeta!}{\lambda!(\lambda+\zeta)!}(\frac{1}{4})^\lambda \partial_z^{[2\lambda]}\Psi_\zeta\ . \tag{13}$$

For an arbitrary curvature Γ a recursion formula can also be derived [3]. Therefore the multipole coefficients $\Psi_\zeta(z)$ uniquely characterize the expansion (10) provided they are analytic functions of z.

4 The magnetic vector potential

The relation between a specific vector potential $\vec{A}^*(\vec{r})$ and the scalar potential $\psi(\vec{r})$ follows from the identity

$$\vec{B}(\vec{r}) = \nabla \times (\vec{A}^*(\vec{r}) + \nabla\Lambda(\vec{r})) = -\nabla\psi(\vec{r}) \tag{14}$$

where $\Lambda(\vec{r})$ denotes an arbitrary real scalar gauge function. Using the complex notation, the z-component of the magnetic field $\vec{B}(\vec{r})$ has the form

$$B_z = -\frac{1}{h}\partial_z\psi = -2\Im\{\partial_{\bar{w}}(\bar{A}^* + 2\partial_w\Lambda)\} = 2\Re\{i\partial_{\bar{w}}(\bar{A}^* + 2\partial_w\Lambda)\} \tag{15}$$

with $A^* = A_x^* + iA_y^*$. For an arbitrary real scalar function $\chi(\vec{r})$ the gauge function will be chosen such that

$$-\frac{1}{h}\partial_z\chi = 2\Im\{i\partial_{\bar{w}}(\bar{A}^* + 2\partial_w\Lambda)\} \tag{16}$$

which implies that the gauge function satisfies

$$4\partial_w\partial_{\bar{w}}\Lambda = -\frac{1}{h}\partial_z\chi - 2\Re\{\partial_{\bar{w}}\bar{A}^*\} \ . \tag{17}$$

With this choice of gauge we obtain from equation (14)

$$-\frac{1}{h}\partial_z(\psi + i\chi) = 2i\partial_{\bar{w}}\bar{A} \ , \tag{18}$$

$$2ih\partial_w\psi = -\partial_z\bar{A} + 2\partial_w(hA_z) \ . \tag{19}$$

Here $\vec{A} = \vec{A}^* + \nabla\Lambda$ denotes the vector potential in the new gauge. We choose $\chi(\vec{r})$ as an arbitrary solution of the Laplace equation

$$2\partial_w\{h\partial_{\bar{w}}(\psi + i\chi)\} + 2\partial_{\bar{w}}\{h\partial_w(\psi + i\chi)\} + \partial_z\{\frac{1}{h}\partial_z(\psi + i\chi)\} = 0 \ . \tag{20}$$

The linear combination $\Pi = \psi + i\chi$ has been defined as complex scalar potential [2]. Here we want to stress the crucial point $\Im\{\nabla^2\Pi\} = 0$. Only because of the specific choice (17) of the gauge function we were able to deduce the simple equation (18) which can be integrated directly:

$$\bar{A} = \frac{i}{2}\int_0^{\bar{w}} \frac{1}{h}\partial_z(\psi + i\chi)d\bar{w} + f(z, w) \tag{21}$$

where f is an arbitrary function which does not depend on $\bar{w}$. Inserting $\bar{A}$ into equation (19) and employing the Laplace equation (20), we obtain

$$\begin{aligned}
\partial_w(hA_z) &= ih\partial_w\psi + \frac{i}{4}\int_0^{\bar{w}}[-2\partial_w\{h\partial_{\bar{w}}(\psi+i\chi)\} - 2\partial_{\bar{w}}\{h\partial_w(\psi+i\chi)\}]d\bar{w} \\
&+ \frac{1}{2}\partial_z f(z,w)\ . \qquad (22)
\end{aligned}$$

This relation can be directly integrated over w. The boundaries of the integration must be taken into account very carefully by considering relations such as $\int_0^{\bar{w}}\partial_{\bar{w}}\{h\partial_w(\psi+i\chi)\}d\bar{w} = h\partial_w(\psi+i\chi) - [h\partial_w(\psi+i\chi)]_{\bar{w}=0}$. Moreover, the order of integration with respect to w and $\bar{w}$ must be exchanged. As a result we find

$$\begin{aligned}
hA_z &= i\int_0^{w} h\partial_w\psi dw - \frac{i}{2}\int_0^{w}\{h\partial_w(\psi+i\chi) - [h\partial_w(\psi+i\chi)]_{\bar{w}=0}\}dw \\
&- \frac{i}{2}\int_0^{\bar{w}} h\partial_{\bar{w}}(\psi+i\chi)d\bar{w} + \frac{1}{2}\int_0^{w}\partial_z f(z,w)dw + g(z,\bar{w})\ . \qquad (23)
\end{aligned}$$

Integrating by parts and inserting the definition (5) of h yields

$$\begin{aligned}
hA_z &= ih\psi - \frac{i}{2}\{h(\psi+i\chi) - [h(\psi+i\chi)]_{\bar{w}=0}\} - \frac{i}{2}\int_0^{\bar{w}}\partial_{\bar{w}}\{h(\psi+i\chi)\}d\bar{w} \\
&+ \frac{i}{2}\bar{\Gamma}\int_0^{w}\psi dw - \frac{i}{4}\bar{\Gamma}\int_0^{w}\{(\psi+i\chi) - [\psi+i\chi]_{\bar{w}=0}\}dw \\
&- \frac{i}{4}\Gamma\int_0^{\bar{w}}(\psi+i\chi)d\bar{w} + \frac{1}{2}\int_0^{w}\partial_z f(z,w)dw + k(z,\bar{w}) \qquad (24)
\end{aligned}$$

where $g(z,\bar{w})$ and $k(z,\bar{w})$ are arbitrary analytical functions of z and $\bar{w}$. By rearranging the terms on the right-hand side we obtain

$$\begin{aligned}
hA_z &= h\chi + \frac{1}{2}\frac{1}{2i}\{\Gamma\int_0^{\bar{w}}(\psi+i\chi)d\bar{w} - \bar{\Gamma}\int_0^{w}(\psi-i\chi)dw\} \\
&+ i[h(\psi+i\chi)]_{\bar{w}=0} + \frac{i}{4}\bar{\Gamma}\int_0^{w}[\psi+i\chi]_{\bar{w}=0}dw
\end{aligned}$$

$$+ \quad \frac{1}{2}\int\limits_0^w \partial_z f(z,w)dw + k(z,\bar{w}) \ . \tag{25}$$

The arbitrary functions f and k must be chosen in such a way that the right-hand side of (25) is a real function. The part

$$i[h(\psi + i\chi)]_{\bar{w}=0} + \frac{i}{4}\bar{\Gamma}\int\limits_0^w [\psi + i\chi]_{\bar{w}=0} dw \tag{26}$$

is only a function of z and w. Therefore $k(z,\bar{w})$ can be chosen to be the complex conjugate of this function. It is not possible to simplify the expressions with another choose than $f = 0$. With this we obtain

$$\bar{A} \ = \ \frac{i}{2}\int\limits_0^{\bar{w}} \frac{1}{h}\partial_z(\psi + i\chi)d\bar{w} \ , \tag{27}$$

$$\begin{aligned} hA_z \ &= \ h\chi + \frac{1}{2}\Im\{\Gamma\int\limits_0^{\bar{w}}(\psi + i\chi)d\bar{w}\} \\ &- \ 2\Im\{[h(\psi + i\chi)]_{\bar{w}=0}\} - \frac{1}{2}\Im\{\bar{\Gamma}\int\limits_0^w [\psi + i\chi]_{\bar{w}=0}dw\} \ . \end{aligned} \tag{28}$$

With the knowledge of the magnetic vector potential and equation (2) we can compute the eikonal by integrating along a path $\vec{s}(z)$ that starts at $\vec{s}(z_0)$:

$$S = \int_{\text{path}} (m\vec{v} + q\vec{A})d\vec{s} = m_0 c \int\limits_{z_0}^{z} \mu(z)dz \tag{29}$$

with the rest mass m_0. The right-hand side defines the variational function:

$$\mu(z) = \frac{1}{m_0 c}(mv + q\vec{A}\vec{t})\frac{ds}{dz} \tag{30}$$

with the differential path length $ds = |d\vec{s}|$ and the tangent $\vec{t} = d\vec{s}/ds$. In complex notation the path is described by $w(z), \bar{w}(z)$ such that the variational function is written

$$\mu = \frac{mv}{m_0 c}\sqrt{h^2 + w'\bar{w}'} + \frac{q}{m_0 c}(\Re\{w'\bar{A}\} + hA_z) \tag{31}$$

with $w' = dw/dz$. Because of the equations (27) and (28) this is equivalent to

$$\begin{aligned}
\mu &= \frac{mv}{m_0 c}\sqrt{h^2 + w'\bar{w}'} \\
&+ \frac{q}{m_0 c}[h\chi - \frac{1}{2}\Im\{w' \int\limits_0^{\bar{w}} \frac{1}{h}\partial_z(\psi + i\chi)d\bar{w}\} \\
&+ \frac{1}{2}\Im\{\Gamma \int\limits_0^{\bar{w}} (\psi + i\chi)d\bar{w}\} - 2\Im\{[h(\psi + i\chi)]_{\bar{w}=0}\} \\
&- \frac{1}{2}\Im\{\bar{\Gamma} \int\limits_0^{w} [(\psi + i\chi)]_{\bar{w}=0} dw\}] \ . \qquad (32)
\end{aligned}$$

The advantage of the formulas (27), (28) and (32) arises from the fact that no integration over the path length z is required. The necessary integrations with respect to w and $\bar{w}$ are straightforward integrations of Taylor series which can be performed to arbitrary order by formula manipulators or DA programs.

Since the only constraint on the function $\chi(\vec{r})$ is that it has to fulfill the Laplace equation this function can be expanded in a series of plane multipoles whose coefficients $\chi_\zeta(z)$ can be chosen arbitrarily. With definition (10) and (11) we get

$$[\psi + i\chi]_{\bar{w}=0} = \frac{1}{2}\sum_{\zeta=1}^{\infty}(\bar{\Psi}_\zeta + i\bar{\chi}_\zeta)w^\zeta + \Psi_0 \qquad (33)$$

where it was considered that Ψ_0 is real. The following choice simplifies the expansion for $\vec{A}$:

$$\chi_\zeta = -i\Psi_\zeta \text{ for } \zeta \neq 0,\ \chi_0 = 0 \quad \Rightarrow \quad [\psi + i\chi]_{\bar{w}=0} = \Psi_0 \qquad (34)$$

which yields:

$$\begin{aligned}
\bar{A} &= \frac{i}{2}\int\limits_0^{\bar{w}} \frac{1}{h}\partial_z(\psi + i\chi)d\bar{w} \ , \qquad (35) \\
hA_z &= h\chi + \frac{1}{2}\Im\{\Gamma \int\limits_0^{\bar{w}} [(\psi + i\chi) - \Psi_0]d\bar{w}\} \ .
\end{aligned}$$

For the chosen gauge (34) the expansion of the complex scalar potential in plane multipoles has the form

$$
\begin{aligned}
\Pi = \psi + i\chi &= \Psi_0 \\
&+ \Psi_1 \bar{w} \\
&+ \Psi_2 \bar{w}^2 + \frac{1}{4}(\Psi_1 \bar{\Gamma} - \Psi_0'') w\bar{w} \\
&+ \Psi_3 \bar{w}^3 + \frac{1}{8}(2\Psi_2 \bar{\Gamma} - \Psi_1'') w\bar{w}^2 \\
&+ \frac{3}{16}\Psi_1 \Re\{\Gamma w \bar{w}^2\}\bar{\Gamma} - \frac{1}{16}\Re\{(5\Psi_0''\Gamma + 2\Psi_0'\Gamma') w\bar{w}^2\} \\
&+ \dots \,.
\end{aligned} \tag{36}
$$

This expansion corrects equation (54) of [2]. Since the incorrect expression for the complex scalar potential has been used in that publication, equation (60) and (61) of [2] are also erroneous and must be replaced by the correct formulas for the components of the magnetic vector potential:

$$
\begin{aligned}
\bar{A} &= \frac{i}{2}[\Psi_0' \bar{w} \\
&+ \frac{1}{2}\{(\Psi_1' + \frac{1}{2}\Psi_0'\Gamma)\bar{w}^2 + \Psi_0'\bar{\Gamma} w\bar{w}\} \\
&+ \frac{1}{12}(4\Psi_2' + 2\Psi_1'\Gamma + \Psi_0'\Gamma^2)\bar{w}^3 + \frac{1}{4}\Psi_0'\bar{\Gamma}^2 w^2\bar{w} \\
&+ \frac{1}{8}(\Psi_1\bar{\Gamma}' + 3\Psi_1'\bar{\Gamma} + 2\Psi_0'\Gamma\bar{\Gamma} - \Psi_0''')w\bar{w}^2] \\
&+ \dots \,,
\end{aligned} \tag{37}
$$

$$
\begin{aligned}
hA_z &= \Im\{\Psi_1 \bar{w}\} \\
&+ \Im\{(\Psi_2 - \frac{1}{4}\Psi_1\Gamma)\bar{w}^2 - \frac{1}{4}\Psi_1\bar{\Gamma} w\bar{w}\} \\
&+ \Im\{(\Psi_3 - \frac{1}{3}\Psi_2\Gamma)\bar{w}^3 \\
&\quad + \frac{1}{32}(-8\Psi_2\bar{\Gamma} + \bar{\Psi}_1\Gamma^2 + \Psi_1\Gamma\bar{\Gamma} - 4\Psi_1'' - 2\Psi_0''\Gamma)w\bar{w}^2\} \\
&+ \dots \,.
\end{aligned} \tag{38}
$$

The gauge $\chi = 0$ yields the simplest variational function:

$$
\mu = \frac{mv}{m_0 c}\sqrt{h^2 + w'\bar{w}'} - \frac{q}{m_0 c}[\frac{1}{2}\Im\{w' \int_0^{\bar{w}} \frac{1}{h}\partial_z \psi d\bar{w}\} \tag{39}
$$

$$- \quad \frac{1}{2}\Im\{\Gamma \int_0^{\bar{w}} \psi d\bar{w}\} + \frac{1}{2}\Im\{\bar{\Gamma} \int_0^{w} [\psi]_{\bar{w}=0} dw\} + 2\Im\{[h\psi]_{\bar{w}=0}\}] \ .$$

With this formula μ can be computed to order $n+1$ if the multipole expansion of scalar potentials is known to order n. The reason for this fact is that the $(n+1)^{th}$ order expansion of $[h\psi]_{\bar{w}=0}$ is trivially

$$[h\psi]_{\bar{w}=0} = (1 - \frac{1}{2}\bar{\Gamma}w)(\frac{1}{2}\sum_{\zeta=1}^{\infty} \bar{\Psi}_\zeta w^\zeta + \Psi_0) \ . \tag{40}$$

Of course, the variational function of the eikonal method depends on the choice of the function $\chi(\vec{r})$ because the Lagrangian is not gauge invariant. Nevertheless, it was proved in [7] that the transfer function or map from the initial to the final plane, calculated by the eikonal method, does not depend on the gauge.

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Figure caption

Figure 1: a) The curvilinear coordinate system, b) derivation of the metric coefficient $g_3 = |d\vec{r}/dz|$ at a point where the reference curve has a curvature of $1/\rho$.