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Lens theory of non-paraxial rays for electron gun characterization

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Abstract

It has been attempted to characterize the cathode rays inside electron guns by utilizing the optical concepts familiar in the paraxial lens theory. We have proposed the Canonical Mapping Transformation (CMT) theory to obtain the gun optical parameters. The method is based on the Lagrange differential invariant theorem known in analytical mechanics. It has been found that major electron source properties, such as the crossover position, crossover size, and the angular current intensity, are all deducible from the four CMT optical parameters ($z_{co}$, $f$, $C_{sg}$, and $C_{cg}$), which in turn can be estimated by calculating the normal electron rays, whose emanation vectors on the cathode surface are in the surface normal direction. Since the normal electron rays can in many cases be regarded as paraxial, a scheme has been proposed to calculate the relevant optical parameters by a modification of the conventional paraxial trajectory calculation. It is shown that the normal electron ray of the CMT theory corresponds to $(1, 0)$ principal trajectory in the paraxial method, $g(z)$. The conventional perturbation characteristic function integral method can be employed for the evaluation of the CMT aberration coefficients. Two realistic electron gun models (a single-crystal LaB6 cathode gun and a Schottky emitter source) were analyzed by use of the CMT optical parameters. Both the ray tracing of the normal electrons and the modified paraxial calculation method were employed for the analyses. It has been found that the guns with quite different nature in the source properties can well be described by the CMT optical parameters proposed. The paraxial calculations have been shown to produce accurate enough results and the authors hope their use would help electron optical column designers both in reducing the work load and in having clear physical images of their gun characteristics.

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1. Introduction

In the designing process of electron optical columns (EOCs) such as TEMs, SEMs, and microfocus X-ray tubes, simulation software packages are now extensively used. One major reason the EOC analysis programs is so useful in the designing is that they offer the results in the form of the optical parameters that can be easily interpreted by

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the designers on the basis of a well established theory, the paraxial trajectory theory. One can form a clear physical image of the column in terms of the principal optical parameters like focal lengths, principal plane positions, and magnification factor as well as of several aberration coefficients which prescribe deviations of the system’s behaviour from the linear formula. It should be emphasized that those simulation software packages are not only ray-tracing the electron trajectories in the electrostatic/magnetic field, but they also provide the physical image by offering the results in the form of the optical parameters.

It has been generally accepted that the paraxial trajectory theory cannot directly be applied to the cathode rays inside the electron gun. The starting angle of electrons from the cathode surface can be as large as \( \pi/2 \) with respect to the optical axis and it is evident that the theory breaks down from the beginning in its conventional form. Hence one cannot use the optical concepts familiar in the paraxial lens theory and has to struggle with many cathode rays calculated by direct ray tracing in extracting the gun property. The interpretation of the results is not always straightforward and in some cases one needs to be worried about the fact that the ray-tracing calculation may not be accurate enough for evaluating electron sources with very small virtual crossovers like those encountered in field emitters.

However, if one looks, for example, at the crossover formation of a triode gun as shown in Fig. 1, it is noticed that the source properties are still determined by the ray conditions (the trajectory coordinates and its slope) at the back focal plane. It is then hoped that the use of the optical concepts familiar in the paraxial trajectory theory somehow be extended to non-paraxial cathode rays. Then there might be a possibility that the relevant source properties, such as crossover size and angular current intensity, can be obtained by calculating only a few principal rays and deriving an appropriate set of optical parameters from them. That would make the characterization of electron guns a clearer and, hopefully, much more efficient process.

![Fig. 1. An example of the crossover formation of a triode gun. Even with electron guns, the source properties are determined by the ray conditions (the trajectory coordinates and its slope) at the back focal plane.](image)

That is the hope with which the authors have been trying to establish the “lens theory for non-paraxial rays,” which was named Canonical Mapping Transformation (CMT) theory [1]. In the present article, we shall first explain the mathematical essence of the CMT theory and then introduce the optical parameters useful in characterizing the electron source properties. Those optical parameters will be shown, in many cases, to be calculable with the conventional paraxial trajectory method if a minor modification is made. Interpreting the optical parameters in the
context of CMT theory, one can grasp the crossover property of electron guns. Finally a few applications to realistic electron gun models will be presented to demonstrate the power of the CMT theory to give a clear physical image of the gun with different nature.

2. CMT theory

2.1. CMT diagram

Figure 2(a) shows the CMT ray condition parameters: \( \xi \) and \( \eta \) are the coordinates of ray intersection points measured along the equipotential reference surfaces and \( u = \sin \alpha \) and \( v = \sin \beta \) are the sines of the ray angles \( \alpha \) and \( \beta \) from the respective surface normals. Note that the coordinate \( \eta \) is an asymptote traced back from the field free region. The CMT theory describes the relationship between the ray condition on the cathode surface (\( \xi, u \)) to that in the crossover plane (\( \eta, v \)). The CMT diagram is a 2-dimensional mapping from the CMT variables (\( \xi, u \)) to (\( \eta, v \)). An example of the diagram is shown in Fig. 2(b). It is drawn from the ray-tracing results of a model triode electron gun presented in Fig. 3, which is composed of a flat cathode, a Wehnelt electrode and an anode. The applied voltages assumed in the ray-tracing were \( V_{\text{cathode}} = 0 \text{V}, V_{\text{anode}} = 5000 \text{V}, \) and \( V_{\text{Wehnelt}} = -484 \text{V} \) (the cutoff voltage is \( V_{\text{cutoff}} = -564 \text{V} \)). A fixed initial electron energy of \( E_0 = 0.2 \text{eV} \) was assumed. All the ray tracing presented in this article was computed using CPO program [2].

It is readily noted that the CMT diagram is closely related to the emittance diagram widely used in presenting electron gun source properties. The ordinate axis used in the CMT diagram is not the tangent of the ray angle but the sine of it. However, since the emerging rays from the electron guns usually make small angle with respect to the axis the difference is not important (note that \( \tan(0.1 \text{ rad}) = 0.1003 \) compared with \( \sin(0.1 \text{ rad}) = 0.0998 \)).

While the conventional emittance diagram is usually calculated with varied ray initial conditions on the cathode to represent actual distribution of electron velocities and its purpose is to simulate the emittance intensity distribution, the CMT diagram assumes a specific set of initial condition and its role is to relate the initial ray condition on the cathode to that at the crossover plane. If a simple relation can be found between the two ray conditions, tedious task of actually ray-tracing many cathode rays with various initial conditions will be made unnecessary in obtaining the emittance.

The CMT diagram in Fig. 2(b) indicates that area of each \( \Delta \xi \times \Delta u \) element enclosed by grids is the same. The fact is rigorously satisfied by general non-paraxial rays and is a consequence of the Lagrange differential invariant theorem [1]. The Lagrange bracket relation must be satisfied by general non-paraxial rays and is given by the following equation, when expressed in terms of the CMT variables,

\[
J = \frac{\partial \eta_v}{\partial \xi u} \frac{\partial \eta_v}{\partial \xi u} - \frac{\partial \eta_u}{\partial \xi v} \frac{\partial \eta_u}{\partial \xi v} = \frac{\Phi_0}{\Phi_1},
\]

where \( \Phi_0 \) and \( \Phi_1 \) are the initial and accelerated electron energies measured in electron-volts. Equation (1) guarantees that each \( \Delta \xi \times \Delta u \) element in the CMT diagram has the same area.

2.2. CMT optical parameters

Because the Lagrange bracket relation (1) must be satisfied, it is possible to characterize the transformation by a small number of parameters. Let’s start with a linear approximation. A simple calculation shows the linear approximation of the 2-dimensional (2D) transformation compatible with the Lagrange bracket relation (1) is given by

\[
\eta_\xi(\xi, u) = f \sqrt{\Phi_0/\Phi_1} u
\]

\[
v(\xi, u) = -\xi/f + mu.
\]
Here use is made of the fact the crossover coordinate $c_K$ is independent of the cathode coordinate $[\text{in the linear approximation according to the way the crossover plane is defined. As the CMT diagram in Fig. 2(b) demonstrates, the crossover position is so defined that the ray $(\eta_c, v = \sin \beta)$ points for the normal electron rays, with the initial condition $u = \sin \alpha = 0$, will be aligned vertically in the diagram. Equations (2) and (3) show only two optical parameters, $f$ and $m$, are necessary to specify the transformation in addition to the acceleration ratio $\Phi_1/\Phi_0$. The conventional ray definition using the tangents instead of the sines is not convenient to be compatible with the CMT condition (1). Any linear transformations expressed in the conventional ray variables do not satisfy Eq. (1); large higher-order terms are inevitably introduced as aberrations. In contrast, one can expect that the higher-order aberration terms may be small if one adopts CMT variables for the ray definition.

Fig. 2. (a) The CMT ray variables. In the CMT theory the ray conditions on the cathode surface $(\xi, u = \sin \alpha)$ is related to those in the crossover plane $(\eta_c, v = \sin \beta)$. Here, $\xi$ and $\eta_c$ are the coordinates of ray intersection points measured along the equipotential reference surfaces and $u$ and $v$ are the sines of the ray angle with respect to the surface normal. (b) An example of the CMT diagram. The CMT diagram is a 2-dimensional mapping from the CMT variables $(\xi, u = \sin \alpha)$ to $(\eta_c, v = \sin \beta)$. It is drawn from the ray-tracing results of a model triode electron gun.

Fig. 3. A model triode electron gun used in the explanation of the CMT theory, which is composed of a flat cathode, a Wehnelt electrode, and an anode. The ray tracing and paraxial trajectory calculation will be performed on this model gun and the results compared.

Here use is made of the fact the crossover coordinate $\eta_c$ is independent of the cathode coordinate $\xi$ in the linear approximation according to the way the crossover plane is defined. As the CMT diagram in Fig. 2(b) demonstrates, the crossover position is so defined that the ray $(\eta_c, v)$ points for the normal electron rays, with the initial condition $u = \sin \alpha = 0$, will be aligned vertically in the diagram. Equations (2) and (3) show only two optical parameters, $f$ and $m$, are necessary to specify the transformation in addition to the acceleration ratio $\Phi_1/\Phi_0$. The conventional ray definition using the tangents instead of the sines is not convenient to be compatible with the CMT condition (1). Any linear transformations expressed in the conventional ray variables do not satisfy Eq. (1); large higher-order terms are inevitably introduced as aberrations. In contrast, one can expect that the higher-order aberration terms may be small if one adopts CMT variables for the ray definition.
Especially important is the parameter, *electron gun focal length* \( f \). It is defined by the *normal electron rays* that are emitted perpendicularly from the cathode surface. Equation (3) directly suggests the mathematical definition given below:

\[
\frac{1}{f} = \lim_{\alpha \to 0} \left( -\frac{\partial \gamma}{\partial \xi} \right) = \lim_{\alpha \to 0} \left( -\frac{\partial \sin \beta}{\partial \xi} \right) .
\] (4)

Fig. 4(a) gives a graphical representation of Eq. (4). Note that in order to estimate \( f \) there is no need to calculate inclined rays that start from the cathode with finite emission angles. In the example shown in Fig. 2(b) the focal length was evaluated to be \( f = 1.65 \text{ mm} \). The electron gun focal length is an extended concept of the image side focal length in the conventional lens theory. The correspondence is obvious if one compares the graphical definitions of the two focal lengths given in Figs. 4(a) and 4(b), respectively.

Then Eq. (2) shows the crossover coordinate \( \eta \) of an inclined ray is, in good approximation, proportional to the sine of the ray starting angle \( u = \sin \alpha \) and the proportionality coefficient is given by the electron gun focal length. In the case of the example gun, the crossover coordinate of the inclined ray starting from the center \( \xi = 0 \) with \( \alpha = \pi/2 \) was calculated by ray tracing to be \( \eta = 10.2 \mu \text{m} \), which should be compared with the linear approximation result (2), \( \eta = 1650 \sqrt{0.2/5000} \cdot 1 = 10.4 \mu \text{m} \). The agreement is very satisfactory even with linear approximation. In principle the electron gun focal length is defined for each initial energy. But it was found that it depends only slightly on the energy except for the cases where the electric field on cathode surface is extremely weak. Its independence of the
initial energy makes the crossover property evaluation substantially simpler since one has only to calculate the electron gun focal length for a single initial energy and use the result for the entire range of electron initial energy distribution. Consequently, simple formulas can be obtained for the crossover size $d_{co}$ and the angular current intensity $J_{\alpha}$ in terms of the electron gun focal length$^a$:

$$d_{co} = 2f \sqrt{\frac{kT}{e\Phi_i}}$$

$$J_{\alpha} = f^2 j, \quad \text{(6)}$$

where $T$ is the cathode temperature representing the initial tangential energy spread of electrons and $j$, the cathode current density [1].

2.3. Gun aberrations

So far we have been concerned with the axial property of the CMT diagram. The crossover size evaluated by Eq. (5) is the one that would be obtained with a sufficiently small acceptance angle. When the acceptance angle is made larger, the beam size in general increases due to the gun spherical aberration effect. Here we denote by the gun spherical aberration the S-shape curvature of the CMT diagram (see Fig. 2(b)). The value of the spherical aberration coefficient, $C_{sg}$, is obtained by fitting the crossover coordinate $\eta$, for normal electrons rays ($u = \sin \alpha = 0$) by a third order polynomial of the cathode coordinate $\xi$,

$$\eta_{ss}(\xi, u = 0) = -C_{sg}(\xi/f)^3. \quad \text{(7)}$$

The spherical aberration defined here has the same effect in beam blurring as that of the probe-forming lens. The apparent crossover size increase with the beam acceptance angle $\beta$ due to the gun spherical aberration can be estimated by:

$$d_{gs} = \frac{1}{2} C_{sg} \beta^3,$$

where it is assumed that the angle $\beta$ is small enough as is usually done in electron optics.

Another aberration effect that should be taken into account but is not explicitly represented in the CMT diagram in Fig. 2(b) is the gun chromatic aberration. This aberration is due to the shift of the crossover position with the electron initial energy. The crossover plane is defined by the normal electron rays as the plane where they converge and the linear dependence of the crossover coordinate $\eta$, on the initial cathode coordinate $\xi$ vanishes. The crossover position $z_{co}$ is a function of the initial energy $E_0$ and the gun chromatic aberration coefficient $C_{cg}$ is defined by:

$$C_{cg} = \Phi_1 \frac{\partial z_{co}}{\partial E_0}, \quad \text{(9)}$$

where multiplication by the acceleration voltage $\Phi_1$ implies the coefficient is defined with respect to the accelerated beam energy. The effect of the beam blurring by the gun chromatic aberration, $d_{cg}$, is given by the same formula as is used in probe forming lens:

$$d_{cg} = C_{cg} \frac{\Delta \Phi}{\Phi_1} \beta. \quad \text{(10)}$$

$^a$ The crossover size given here by Eq. (5) assumes the Gaussian current density distribution and it is given by the full width at 1/e maximum. The Gaussian type current distribution is valid both in thermionic cathode guns and the Schottky emitter sources if we can ignore the influence of the aberrations. However, there are arguments on how the source size should be defined (see, for example, Barth J.E. and Kruit P., Optik 101, 101 (1996)). In order to correlate the source size with the image resolution in the presence of the aberration effect to the current distribution, it is argued that the diameter of the circle that contains FC equal to 50%, 75% or any other fraction of the total probe current should be used.
Here, $\Delta \Phi$ is the electron energy spread measured in electron volts.

The CMT theory suggests that the electron source properties as represented in the CMT diagram can be summarized in terms of only a few CMT parameters. We can conclude from the arguments above that four optical parameters usually suffice to characterize electron gun properties. They are 1) electron gun focal length $f$, 2) crossover position $z_{co}$, 3) gun spherical aberration $C_{sg}$, and 4) gun chromatic aberration $C_{cg}$. The four CMT optical parameters can be evaluated by fitting the ray-tracing results of the normal electrons to the appropriate formulas given in this section. We designate this parameter derivation as “ray-fitting” method. A method of evaluating the probe property (the relation between the beam current and the final probe size) of an entire electron optical column comprising the gun as well as the lens system by use of the four gun optical parameters was reported in the literature [4].

The arguments above have been confined to the meridional rays but the generalization of the CMT theory to non-meridional skewed rays which is necessary for the study of the electron gun with superimposed magnetic field is straightforward. We have only to extend the 2-dimensional CMT variables to 4-dimensional variables in the ray condition definition in order to take both the x and y components into consideration. The details of the generalized CMT theory was reported elsewhere [5].

3. Calculation of CMT parameters by paraxial trajectory method

The four important gun optical parameters, i.e. the electron gun focal length, the crossover position, and the gun spherical/chromatic aberration coefficients, discussed above are all defined by normal electron rays only. In many cases the normal electron rays can be regarded as paraxial and conventional paraxial trajectory methods can be invoked in their calculation.

We have pointed out in the previous section the correspondence between the electron gun focal length in the CMT theory and the image side focal length in the conventional lens theory. Figure 4 indicates the normal electron ray corresponds to the (1, 0) principal trajectory in the paraxial theory, $g(z)$, which has as its initial condition $g(z_0) = 1$ and $g'(z_0) = 0$. Hence the ray-tracing of the normal electron ray can be substituted by the calculation of $g(z)$ principal trajectory in the paraxial trajectory method. Even the aberration coefficients will be shown to be obtainable by use of the conventional aberration integral method if the integral range is correctly chosen to be from the object plane to the back focal plane, instead of the image plane.

3.1. Formulation of CMT polynomial expansion with aberration terms

We shall explain a method for calculating the CMT diagram with up to the third order geometrical aberrations and the first order chromatic aberrations on the basis of the paraxial trajectory method, thus generalizing the linear approximation formula given in Eqs. (2) and (3). All the aberration terms will be simultaneously calculated in addition to the axial aberration coefficients, $C_{sg}$ and $C_{cg}$.

We shall here explain only the method for calculating the geometrical aberration coefficients of the CMT. The chromatic aberration calculation can be conducted, following almost the same procedures. It is based on the third order polynomial approximation of the CMT:

$$
\eta_i(\xi, u) = \tilde{f} \left[ \Phi_{i0}/\Phi_{i1}u + \sum_{i,j,k,l} a_{ijkl} \xi^i u^j u^l \right] (11)
$$

$$
\nu(\xi, u) = -\xi f/m_0u + \sum_{i,j,k,l} b_{ijkl} \xi^i u^j u^l. (12)
$$
Here we have extended the CMT to 4-dimensional (4D) mapping taking both the \(x\) and \(y\) components of the ray condition variables in the form of complex numbers as in \(\tilde{\xi} = \xi + i\tilde{\xi}\). The upper bar denotes taking complex conjugate. Comparison of Eq. (11) with Eq. (7) shows that the gun spherical aberration coefficient is given by \(C_{e} = f'a_{2100}\). The other third order terms give non-axial aberrations whose forms, as we shall see below, coincide with those of the conventional lens geometrical aberrations. Equation (12) gives the aberrations in the trajectory slope, which can sometimes be important in evaluating the CMT or emittance diagrams.

In evaluating the coefficients, \(a_{ijkl}\) and \(b_{ijkl}\), we first digress from the CMT variables and work with the conventional paraxial trajectory nomenclatures. The “principles of the least action” dictates the paraxial trajectory equations and the aberration formulation. The trajectories are given by the condition that the action integral,\(S = \int \sqrt{2m}e\phi(r,z)\sqrt{1 + x'^2 + y'^2} - e(x'A_x(r,z) + y'A_y(r,z) + A_z(r,z))}\)\(dz\), (13)
is minimized. Here, \(e\) and \(m\) represent, respectively, electron charge and mass, and \(\phi(r,z)\) and \(A_i(r,z)\) \((i = x, y, and z)\) are the electrostatic scalar potential and the magnetic vector potential. The Taylor expansion of Eq. (13) in \(x, y, x'\) and \(y'\) in increasingly higher orders will enable the derivation of the paraxial trajectory equation and the aberration integral formulas.

The principal paraxial trajectories are given by \((1,0)\) and \((0,1)\) trajectories, \(g(z)\) and \(h(z)\), that have as their initial condition at the object plane \(z = z_0\),\(g(z_0) = 1, g'(z_0) = 0\)\(h(z_0) = 0, h'(z_0) = 1\). (14)

The principal trajectories need to be defined in the rotating frame whose rotation angle with respect to the laboratory frame is given by \(\theta(z) = \sqrt{e/m} \int \frac{B_z(\zeta)}{\Phi(\zeta)} d\zeta\), (15)
where \(B_z(\zeta)\) is the axial magnetic flux density and \(\Phi(\zeta)\) is the axial electrostatic potential. Note that the normal electron ray of the CMT theory in the presence of the magnetic field correctly corresponds with the principal trajectory \(g(z)\) defined in the rotating frame, not with the trajectory which is emitted at the object plane parallel to the optical axis. The details are explained in the literature [5].

The paraxial trajectory \(w(z) = x(z) + iy(z)\) (in the laboratory frame) will be specified by the ray condition at the object plane as follows: \(w(z) = x(z) + iy(z) = \left[\xi g(z) + \bar{\xi} h(z)\right] \exp(i\theta(z))\), (16)
where \(\xi = x_o + iy_o\) and \(\bar{\xi} = x_o' + iy_o'\) are, respectively, the initial coordinates and directions in the rotating frame of the trajectory expressed in complex numbers.

The trajectory condition at the crossover plane \(z = z_f\) can be expressed as the sum of the paraxial and third order aberration contributions. A general expression is given by the following formula:

\[
\left(\begin{array}{c}
\frac{w_f}{w_f' - \frac{1}{2}w_f^2\bar{w}_f}\\
\frac{w_f'}{2} - \frac{1}{2}w_f^2\bar{w}_f
\end{array}\right) = \left(\begin{array}{cc}
G_f & H_f \\
G_f' & H_f'
\end{array}\right) \left(\begin{array}{c}
\bar{\xi} \\
\frac{1}{2}w_o^2w_o' - \frac{1}{8}\frac{e}{\Phi_0}\Phi_0 w_o^2w_o' + \frac{i}{16} \sqrt{\frac{e}{2m}} \frac{B_o^2}{\Phi_0} w_o^2w_o' \\
\frac{\partial V' / \partial \bar{\xi}}{\partial V' / \partial \bar{\xi}}
\end{array}\right)
\]
(17)
where \( H(z) \) and \( G(z) \) are, respectively, the asymptotes to the principal trajectories \( h(z) e^{i\phi} \) and \( g(z) e^{i\phi} \) from the field free region, and \( V^f(\xi, \nu, \xi', \nu') \) is the perturbation characteristic function for the third order geometrical aberrations [6] whose form is given in Appendix A. The subscripts “0” and “f” to the functions indicate taking the function values at \( z = z_0 \) (the cathode surface) and \( z_f \) (the back focal plane) respectively. Even though \( G_f = G(z_f) = 0 \) at the back focal plane by definition, we have chosen to include the term explicitly in order to enable the calculation of the CMT diagram at a defocused position \( z = z_f + \Delta z \).

A comment should be given to terms in the trajectory direction component (the second component in column vectors). The third order terms in the direction components originate from the way in which the momentum is defined as a partial derivative of the action integrand function \( F \) of the system. Equation (18) shows the momentum of a given trajectory with the same coordinate and the gradient does change when higher order terms are taken into consideration in the action integrand function. The third order terms in Eqs. (17) needed to be included in order to account for this change. It can be shown that the sums of the first and third order terms in the directional components are equivalent to the CMT canonical direction \( u \) and \( v \) up to the order concerned; note that \( \xi^0 = w_0^0 - (i/2)(e/2m\Phi_0)^{1/2} B_0^0 w_0^0 \) because of the rotation in the coordinate system. The advantage of the use of the CMT canonical direction parameters \( u \) and \( v \), i.e. the use of the directional sines instead of the tangents, has been reestablished through the aberration formulation in the paraxial trajectory theory. Apparent aberration terms can be renormalized into the CMT canonical direction.

The CMT up to the third order aberrations given in Eqs. (11) and (12) can be obtained from the paraxial trajectory formula, Eq. (17). All one needs to do is first to omit the third order terms in the directional component and then to replace paraxial trajectory parameter \( \xi^p \) with the CMT canonical direction \( u \):

\[
\begin{pmatrix}
\eta = \eta_x + i\eta_y \\
\nu = \nu_x + \nu_y
\end{pmatrix} = \begin{pmatrix}
G_f & H_f \\
G'_f & H'_f
\end{pmatrix} \begin{pmatrix}
\xi = x_0 + i y_0 \\
u = u_x + i u_y
\end{pmatrix} + \begin{pmatrix}
-\partial V^f/\partial \xi^p \\
\partial V^f/\partial \xi^p
\end{pmatrix}.
\]

The obtained transformation is correct up to the third order terms; remember that \( \xi^p \) in the perturbation characteristic function \( V^f(\xi, \nu, \xi', \nu') \) should also be replaced by \( u \). It is straightforward to extract the relevant CMT optical parameters from the paraxial trajectory calculation results.

The calculation of the chromatic aberrations proceeds almost in parallel with the way described above. The only difference is that we now have to use the perturbation characteristic function for the chromatic aberration \( V^c(\omega_0, \bar{\omega}_0, w'_0, \bar{w}'_0) \) whose integration form is also given in Appendix A.

We shall name this optical parameter derivation as the “paraxial calculation” method, to distinguish it from the “ray-fitting” of the normal electrons.
3.2. Accuracy in paraxial trajectory calculations of CMT parameters

We shall now apply the paraxial trajectory calculation method described above to obtain the CMT diagrams and optical parameters in order to prove the validity of the method. The model electron gun is the one shown in Fig. 3, for which the CMT diagram was calculated in Fig. 2(b). The anode voltage of \( V_{\text{anode}} = 5000 \) V and the electron initial energy of \( E_i = 0.2 \) eV are assumed throughout this subsection.

![Diagram of principal paraxial trajectories and CMT diagram](image)

Fig. 5. (a) The principal paraxial trajectories of the model electron gun and the axial potential distribution. The \( g(z) \) principal trajectory shows the formation of the crossover just in front of the Wehnelt electrode.
(b) The CMT diagram reproduced by the paraxial calculation method using the third order polynomial formulas. Each circle in the figure was by the paraxial calculation, which corresponds to a grid intersection point of the superimposed ray-traced CMT diagram.
The corresponding principal paraxial trajectories are shown in Fig. 5(a) together with the axial potential distribution. The $g(z)$ principal trajectory shows the formation of a crossover just in front of the Wehnelt electrode. The CMT diagram was reproduced by the paraxial calculation method using the third order polynomial formulas (11) and (12). The result is presented in Fig. 5(b). Each circle in the figure was by the paraxial calculation, which should ideally fall on grid intersections of the superimposed ray-traced CMT diagram. Agreement looks satisfactory considering that only up to third order terms are taken into account. Let us emphasize the fact that there is no fitting parameters for adjusting the paraxial diagram to the ray-traced CMT diagram. Only information fed to the paraxial calculation is the axial potential distribution.

In Fig. 6 we compare the crossover size obtained by the direct ray tracing (square marks) with that evaluated by Eq. (2) in which the focal length was calculated by the paraxial method (solid curve). The crossover size was estimated as a function of the drive voltage, $V_d = V_{Whehnelt} - V_{cutoff}$. The ray inclination angle used for the crossover size comparison was $\alpha = 53.1$ degree, i.e. $u = 0.8$. The agreement is satisfactory both in the absolute value and in the behaviour as a function of the drive voltage.

The four CMT optical parameters were calculated both by the ray-fitting of the normal electrons and by the paraxial calculation. Figure 7(a) shows the electron gun focal length $f$ and the crossover position $z_{co}$ as a function of the drive voltage. Square marks are the results of the ray-fitting and the solid curves are from the paraxial calculation. The paraxial calculation method gives them as the first order optical parameters. The agreement is quite good except for very low drive voltage range where the Wehnelt voltage is very close to the cutoff and the electron gun focal length depends strongly on the initial energy (see below).

The gun spherical and chromatic aberration coefficients were also calculated and compared. The results are presented in Fig. 7(b). Here again the ray-fitting results are given by the square marks and those by paraxial calculation by solid curves. It was confirmed that the gun axial aberration coefficients can be estimated with good accuracy by the paraxial trajectory method.
Fig. 7. (a) The electron gun focal length $f$ and the crossover position $z_{co}$ as a function of the drive voltage. Square marks are the results of the ray-fitting and the solid curves are from the paraxial calculation.

(b) The gun spherical and chromatic aberration coefficients. They were calculated and compared adopting both the ray-fitting (square marks) and the paraxial calculation (solid curve). The aberration coefficients were evaluated by integrating the perturbation characteristic functions in the paraxial calculation.

We have mentioned in the previous section that the electron gun focal length is in general a function of the electron initial energy $E_0$ but is practically independent of it when the electric field on cathode surface is not very weak. Since its independence would makes analysis of the crossover current distribution substantially simpler, it would be convenient if one could estimate to what extent the electron gun focal length depends on the initial energy within the paraxial calculation scheme.
The paraxial calculation method can provide this dependence because the electron gun focal length is defined by the slope of the (1,0) trajectory (see Fig. 4) and the chromatic aberration of the trajectory slope gives the required information. In Fig. 8 we calculated \( \frac{\partial f}{\partial E_0} \) using paraxial calculation method (solid curve) and compare it with the value obtained from the ray fitting method (square marks), where the focal lengths were actually computed for several initial energies. The estimation results by the two methods agree well with each other. Both results suggest that electron gun focal length depends on the initial energy in low drive voltage range but becomes practically independent of it when the Wehnelt voltage is raised to a certain level to ensure the strong enough electric field on the cathode. In practical gun operation conditions, the focal length can be regarded as independent of the initial energy.

4. Examples

In this section we shall characterize some example electron guns by the CMT method. A LaB6 thermionic cathode gun and a Schottky emitter source have been chosen as representative examples of different types of guns. The CMT diagrams will be calculated both by the direct ray-tracing and by the paraxial calculation method and some important optical parameters are also presented. It will be seen that quite different optical properties of the two electron sources can clearly be characterized in the CMT optical parameters.

4.1. LaB6 thermionic cathode gun properties

A model of the LaB6 cathode gun for use with a microfocus X-ray tube is shown in Fig. 9. While Fig. 9(a) presents the overall construction of the gun, Fig. 9(b) gives an expanded view around the single crystal LaB6 cathode. The dimensions are shown in millimetres. The gun is a triode type and is designed to be operative up to \( V_{\text{anode}} = 160 \text{ kV} \). A feature worth noting is a flat (100) crystal plane on a truncated cone of the cathode whose diameter is 40 \( \mu \text{m} \) (see Fig. 9(b)). Since the work function of the LaB6 (100) plane is lower than those of the other
planes, the electrons can be thought to emanate only from this plane in the first approximation. The half cone angle is 45 degree.

Fig. 9. (a) Overall construction of a model of the LaB6 cathode gun for use with a microfocus X-ray tube. (b) Expanded view around the single-crystal LaB6 cathode. The dimensions are shown in millimetres. The gun is a triode type and is designed to be operative up to $V_{\text{anode}} = 160$ kV.

Fig. 10. (a) The electron gun focal length $f$ and the crossover position $z_{\text{co}}$ of the LaB6 cathode gun as a function of the Wehnelt drive voltage. They were estimated by the paraxial calculation method. The electron gun focal length has a minimum as the Wehnelt voltage is increased from the cutoff, whereas the crossover position shifts forward at the same time. (b) The gun aberration coefficients estimated by the paraxial calculation. A surprising feature of the LaB6 gun aberrations is that they can have negative value.

The electron source properties were evaluated by calculating CMT optical parameters by the paraxial calculation. The anode voltage of $V_{\text{anode}} = 120$ kV was assumed, but the relativistic effect was not taken into consideration in the present calculation. Figure 10(a) shows the principal CMT parameters, i.e. the electron gun focal length $f$ and the crossover position $z_{\text{co}}$, as a function of the Wehnelt drive voltage $V_d (= V_{\text{Wehnelt}} - V_{\text{cutoff}})$. It is clearly shown that the electron gun focal length passes through a minimum as the Wehnelt voltage is increased from the cutoff, whereas...
the crossover position shifts forward at the same time. Equations (5) and (6) show that both the crossover size and angular current intensity are the functions of the electron gun focal length and should take the minimum value where the focal length becomes the shortest.

We have actually observed the change in the angular current intensity in our LaB$_6$ microfocus X-ray tubes which is consistent with the calculation result as the Wehnelt voltage is increased from the cutoff. In some type of microfocus X-ray tubes, only one probe forming lens is used and the system magnification factor is fixed, so it is important to adjust the electron gun operation condition carefully in order to have the smallest possible crossover for achieving the finest probe spot on the target and the highest spatial resolution in X-ray images.

The gun aberration coefficients estimated by the paraxial calculation are shown in Fig. 10(b) as a function of the drive voltage. A surprising feature of the LaB$_6$ gun aberrations is that they can have negative value. When the drive voltage exceeds a certain threshold, the aberrations seem to become negative. In the case of the spherical aberration, it indicates the CMT diagram takes a reversely curved S shape. Is it actually possible?

We have calculated the CMT diagram for the Wehnelt voltage condition of $V_d = 160$ V both by the direct ray tracing and by the paraxial calculation. The electron initial energy of $E_0 = 0.2$ eV was assumed. The results are presented in Fig. 11 in which the ray-tracing result is shown in the form of grids and the paraxial calculation results are presented by circles. The diagram shows, without doubt, the reversely $S$ shaped curve in both the calculation results.

![Fig. 11. The CMT diagram of the LaB6 cathode gun for the Wehnelt voltage condition of $V_d = 160$ V. The diagram was drawn both by the direct ray tracing (grids) and by the paraxial calculation (circles). The electron initial energy of $E_0 = 0.2$ eV was assumed. The diagram shows, without doubt, the reversely $S$ shaped curve, corresponding to the negative spherical aberration.](image-url)
A negative spherical aberration is not prohibited in crossover formations. It was proven impossible by Scherzer in the object-image context in the round lens systems. However, we are now dealing with the object-back focal plane relation and there is no theorem to exclude the negative aberration coefficients. The authors believe that the truncated cone shape of the single-crystal LaB6 cathode is responsible for the negative aberrations, but we are not sure whether there is a practical way to design an electron gun with appropriate negative aberrations, in order to compensate for the lens aberrations. Still, there is at least a possibility.

4.2. Schottky emitter source properties

A simple Schottky emitter source model was evaluated by the CMT method. The calculation model is presented in Fig. 12. Figure 12(a) shows a overall structure, which comprises the emitter, suppressor, extractor, and the anode. The emitter tip shape was faithfully modeled with a (100) plane facet on top as shown in Fig. 12(b). The electrons are emitted solely from the (100) facet where the work function is selectively lowered by the ZrO layer. The suppressor and extractor voltages were set at \( V_{\text{supp}} = -300 \) V and \( V_{\text{ext}} = 4372 \) V, respectively; the extractor voltage was so chosen that there will be electric field of \( F = 1 \times 10^9 \) V/m at the emitter tip, which is about the strength required for extended Schottky-emission operation. An electron initial energy of \( E_0 = 0.155 \) eV was assumed, corresponding to the emitter temperature of \( T = 1800 \) K.

The CMT diagrams were calculated in order to estimate the source properties. Both the direct ray tracing and the paraxial calculation were used and the consistency was checked. In the first calculation the anode voltage was set equal to the extractor voltage, \( V_{\text{anode}} = V_{\text{ext}} = 4372 \) V: there is essentially no field beyond the extractor and source properties are determined by the emitter-suppressor-extractor triode system. The accelerator lens effect by the anode is absent. The calculated CMT diagram is shown in Fig. 13(a). The direct ray-tracing result is presented by the grids and that of the paraxial calculation by the circles. The diagram width represents the source size and it is about \( d = 24.5 \) nm, a value generally accepted for Schottky emitters. The small size of the Schottky emitter source comes from the short focal length, which was calculated to be \( f = -2.05 \) \( \mu \)m, while the focal length of thermionic cathode guns are usually in the range of millimetres. Refer to Eq. (5) for the relation between the source size and the gun focal length. The negative sign of the focal length indicates no real crossover is formed and the beam is divergent. Very small aberrations of the Schottky triode system are remarkable. They were estimated to be in the range of a few tens of micrometers. All the optical parameters presented inside the figure were estimated by the paraxial calculation method. The calculation results of both the ray tracing and the paraxial calculation agree very well. The paraxial calculation result reproduces the detailed features of the diagram caused by the aberration effect.
Fig. 13. (a) The CMT diagrams of the Schottky emitter source calculated by the direct ray tracing (grids) and the paraxial calculation (circles) for the case where the anode voltage was set equal to the extractor voltage, $V_{anode} = V_{ext} = 4372\,\text{V}$. There is no field beyond the extractor. The diagram width represents the source size of $d = 24.5\,\text{nm}$, a value generally accepted for Schottky emitters. The small size of the Schottky emitter source comes from the short focal length. Very small aberrations of the Schottky triode system were remarkable. All the optical parameters presented inside the figure were estimated by the paraxial calculation method.

(b) The CMT diagram of the accelerated source. The anode voltage was increased to $V_{anode} = 10\,\text{kV}$. There is now acceleration lens field between the extractor and the anode. The spherical aberration has now increased to $C_{sg} = 1.00\,\text{mm}$ and the diagram is severely deformed.
In the second calculation, the anode voltage was increased to $V_{\text{anode}} = 10 \text{ kV}$. There is now acceleration field between the extractor and the anode and the lens action takes effect. The influence to the CMT diagram is dramatic. Figure 13(b) shows the CMT diagram of the accelerated source. The spherical aberration has now increased to $C_{sg} = 1.00 \text{ mm}$ and the diagram is severely deformed. The fact shows that one needs to be very careful about the influence of the gun lens aberrations with Schottky emitters. They can deteriorate the source capability quite easily because the original source size is extremely small and the required beam acceptance angle is relatively large.

The agreement between the direct ray-tracing result and the paraxial calculation is not perfect in Fig. 13(b). We believe it is due to the higher order effect. The third order polynomial approximation of the CMT used in Eqs. (11) and (12) may not be accurate enough to reflect the actual field distribution in off-axis volume. The ray tracing shows that some of the off-axial rays come very close to the anode electrode. However, the essential feature in the central portion of the diagram is reproduced well by the paraxial calculation. Since conventional lens effect is automatically taken into account when the paraxial calculation method is adopted in the CMT evaluation of the electron gun properties, it is possible to characterize the whole electron optical column from the emitter through the lens system to the sample by a single calculation. One needs not to combine the ray-tracing result for the electron gun with the paraxial trajectory calculation for the rest of the lens system.

5. Conclusions

It has been attempted to characterize the cathode rays inside electron guns by utilizing the optical concepts familiar in the paraxial lens theory. We have proposed the Canonical Mapping Transformation (CMT) theory for relating the ray condition on the cathode to that at the crossover plane. The method is based on the Lagrange differential invariant theorem known in analytical mechanics. It has been found that major ray characteristics relevant to the electron source properties, such as the crossover position, crossover size and angular current intensity are all deducible from a few CMT optical parameters. The four CMT optical parameters one can obtain by ray-tracing the normal electron rays usually suffice to characterize the electron gun properties: the crossover position $z_{co}$, the electron gun focal length $f$, and the gun spherical/chromatic aberration coefficients, $C_{sg}$ and $C_{cg}$. Practically all the source properties necessary for the designing of electron optical columns are deducible from these four parameters.

A scheme has been proposed to calculate the CMT optical parameters by a modification of the conventional paraxial trajectory method. It has been found that the normal electron ray of the CMT theory corresponds to $(1, 0)$ principal trajectory $g(z)$ of the paraxial method. The conventional perturbation characteristic function method for the evaluation of the aberration coefficients can be employed to calculate CMT aberration coefficients. The modifications are that the sines are used for trajectory direction specification in place of the tangents and that the calculation is now conducted from the object plane to the back focal plane, not to the image plane.

In order to estimate the reliability of the paraxial trajectory method, the CMT (emittance) diagrams and the relevant optical parameters were calculated both by the direct ray-tracing and by the modified paraxial calculation method. The agreements were satisfactory and it has been suggested that the CMT optical parameters can be obtained by the paraxial calculation method, which results in substantial reduction in computation load and leads to offering a clear physical image of the electron gun characteristics.
Two realistic electron gun models (a single-crystal LaB6 cathode gun and a Schottky emitter source) were analyzed by use of the CMT optical parameters. Both the ray tracing and the modified paraxial calculation method were employed for the calculations. It has been found that the guns with quite different nature can well be described in terms of the CMT optical parameters. The paraxial calculation has been shown to produce reliable results and the authors hope its use in the electron gun designing process would help both in reducing the workload and in forming clear physical images of the gun characteristic.

Appendix A. Integration of perturbation characteristic functions

A.1 Geometrical aberration

The perturbation characteristic function for geometrical aberration is given by the following integral:

\[
V^l = \int \frac{\Phi(z)}{\Phi_0} \left[ \frac{1}{128} \left( \Phi^{(4)}(z) - \Phi^{(2)}(z) \right) \right] \left[ r^4 - \frac{\Phi''(z)}{16\Phi(z)} r^2\left(x^2+y^2\right) - \frac{1}{8}\left(x^2+y^2\right)^2 \right] dz
\]

\[
- \left(z_i - z_f\right) \left[ \frac{\Phi_1}{\Phi_0} \frac{1}{8} \left(x_i^2+y_i^2\right)^2 \right]
\]

(A.1)

where \(\Phi_0\) and \(\Phi_1\) are initial and accelerated electron energies (subscript “0” refers to the cathode surface and “1” to the plane at \(z = z_f\) which is located in the field free region) and \(r^2 = x^2 + y^2\). The last subtraction term is necessary to evaluate the aberrations as asymptotic properties at \(z = z_f\).

The perturbation characteristic function \(V^l\) can be expressed in terms of the paraxial trajectory parameters \(\xi\) and \(\xi'\) by substituting into the integral (A.1) the formula for the paraxial trajectory,

\[
w(z) = x(z) + iy(z) = \left[\xi g(z) + \xi' h(z)\right] \exp(i\theta(z)).
\]

(A.2)

The integral and the last subtraction term can be shown to be summarized in the form given below:

\[
V^l(w_0, w_0', w_0', w_0) = \sum_{k=1}^{m} C_k \left[ \Phi_0 \right] g(z), h(z), \theta(z) \right]
\]

(A.3)

where \(C_k\) are the fourth order polynomials whose forms are given in Table A.1 and the functional \(V_k \left[ g(z), h(z), \theta(z) \right]\) is the integral the form of which is given by Eq. (A.1) in which appropriate combinations of \(g(z)\), \(h(z)\), and \(\theta(z)\) should be substituted into the terms \(r^4\), \(r^2(x^2+y^2), (x^2+y^2)^2\), and \(r^2(xy-x'y)\) according to Table A.1.

A.2 Chromatic aberration

The perturbation characteristic function for chromatic aberration is given by the following integral:

\[
V^c = \Delta\Phi \int \frac{\Phi(z)}{\Phi_0} \left[ \frac{1}{16\Phi(z)} r^2 + \frac{1}{4\Phi} \left(x^2+y^2\right) \right] dz - \left(z_i - z_f\right) \left(x_i^2+y_i^2\right)
\]

\[
+ \frac{\Delta(\Lambda N)}{\Lambda N} \left[ \frac{1}{2} \left( \frac{e}{2m\Phi_0} \right) \left( xy' - x'y \right) B_1(z) \right] dz
\]

(A.4)

where \(\Delta\Phi\) represents the electron energy shift and \(\Delta(\Lambda N)\) is the change in lens excitation ampere turns.
We can follow almost the same procedures to express the chromatic perturbation characteristic function in terms of the paraxial trajectory parameters. It is given by the following summation,

\[
V^C(w_o, \overline{w}_o, w'_o, \overline{w}'_o) = \sum_{i=1}^{4} C^C_i \bigg( w_o, \overline{w}_o, w'_o, \overline{w}'_o \bigg) \left[ V^C_i \left[ g(z), h(z), \theta(z) \right] \Delta \Phi + W^C_i \left[ g(z), h(z), \theta(z) \right] \frac{\Delta(NI)}{NI} \right],
\]

where \( C^C_i \left( w_o, \overline{w}_o, w'_o, \overline{w}'_o \right) \) and the combinations of \( g(z), h(z), \) and \( \theta(z) \) which should be substituted into the \( r^2, x^2+y^2, \) and \( xy-x'y' \) terms in the integral (A.4) in the evaluation of the functionals \( V^C_i \left[ g(z), h(z), \theta(z) \right] \) (for energy shift) and \( W^C_i \left[ g(z), h(z), \theta(z) \right] \) (for lens ampere turns change) is listed in Table A.2.

Table A.1
Component list of the geometrical perturbation characteristic function.

| k | \( C^C_i (\xi, \overline{\xi}, \xi', \overline{\xi}') \) | \( r^4 \) | \( r^4(x^2+y^2) \) | \( (x^2+y^2)^2 \) | \( r^2(x'y'-x'y') \) |
|---|---------------------------------|---------|-----------------|-----------------|-----------------|
| 1 | \( \xi^2 \overline{\xi}^2 \) | \( g^2 \) | \( g^2 \left( g^2+\theta^2 \right) \) | \( \left( g^2+\theta^2 \right)^2 \) | \( \theta g^4 \) |
| 2 | \( \xi \overline{\xi} \left( \xi^2+\overline{\xi}^2 \right) \) | \( 2g'h \) | \( g^2 \left( g'h+\theta^2 gh \right) \) | \( 2g^2 \left( g^2+\theta^2 \right) \) | \( 2\theta g^4 \) |
| 3 | \( i\xi \overline{\xi} \left( \xi^2-\overline{\xi}^2 \right) \) | \( \theta g^2 \left( gh-gh' \right) \) | \( 2\theta \left( g^2+\theta^2 \right) \) | \( \frac{1}{2} g^2 \left( gh-gh' \right) \) |
| 4 | \( \xi \overline{\xi} \left( \xi^2 \overline{\xi}^2 \right) \) | \( 2g^2 \) | \( g^2 \left( h^2+\theta^2 \right) \) | \( 2g^2 \left( h^2+\theta^2 \right) \) | \( 2\theta g^4 \) |
| 5 | \( \left( \xi \overline{\xi}+\xi^2 \overline{\xi} \right) \) | \( g^2 \) | \( gh \left( g'h+\theta^2 gh \right) \) | \( \left( g'h+\theta^2 gh \right)^2 \) | \( \theta g^4 \) |
| 6 | \( \left( \xi \overline{\xi}-\xi^2 \overline{\xi} \right) \) | \( \theta \) | \( \right \) | \( \left( gh-gh' \right)^2 \) | \( \right \) |
| 7 | \( i\xi \overline{\xi} \left( \xi^2-\overline{\xi}^2 \right) \) | \( \theta \) | \( \right \) | \( \left( gh-gh' \right)^2 \) | \( \right \) |
| 8 | \( \xi \overline{\xi} \left( \xi^2+\overline{\xi}^2 \right) \) | \( 2gh \) | \( gh \left( h^2+\theta^2 \right) \) | \( 2\theta \left( g'h+\theta^2 gh \right) \) | \( \frac{1}{2} g^2 \left( gh-gh' \right) \) |
| 9 | \( i\xi \overline{\xi} \left( \xi^2-\overline{\xi}^2 \right) \) | \( \theta \) | \( \right \) | \( \left( gh-gh' \right)^2 \) | \( \right \) |
| 10 | \( \xi^2 \overline{\xi}^2 \) | \( h^2 \) | \( h^2 \left( h^2+\theta^2 \right) \) | \( \left( h^2+\theta^2 \right)^2 \) | \( \theta h^4 \) |
Table A.2
Component list of the chromatic perturbation characteristic function.

Each component contained in the expansion of the chromatic perturbation characteristic function is shown. The second column represents the polynomials forms in the trajectory specification coefficients and the third to fifth column each shows the appropriate substitution for the terms in the integral Eq. (A.4) expressed in terms of the principal trajectories.

| k | \( C_k^C \left( \xi, \xi', \eta, \eta' \right) \) | \( r^2 \) | \( x'^2+y'^2 \) | \( xy' - xx' \) |
|---|---|---|---|---|
| 1 | \( \xi \eta' \) | \( g^2 \) | \( g'^2+\theta^2 \) \( g^2 \) | \( \theta g^2 \) |
| 2 | \( \xi \eta + \xi' \eta' \) | \( gh \) | \( g'h+\theta^2 \) \( gh \) | \( \theta gh \) |
| 3 | \( \xi' \xi \) | \( h^2 \) | \( h'^2+\theta^2 \) \( h^2 \) | \( \theta h^2 \) |
| 4 | \( i \left( \xi \eta' - \xi' \eta \right) \) | \( \theta ' \left( g'h - g'h' \right) \) | \( \frac{1}{2} \left( g'h - g'h' \right) \) |

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