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Erwin K. Kasper
Universitaet Auf der Morgenstelle

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RECENT DEVELOPMENTS IN NUMERICAL ELECTRON OPTICS

Erwin K. Kasper

Institut fuer Angewandte Physik
der Universitaet
Auf der Morgenstelle
74 Tuebingen, W. Germany
Phone: 07071/296747
292429

Abstract

The familiar methods for the numerical calculation of fields in electron optical devices are outlined briefly. For the solution of self-adjoint elliptic differential equations in orthogonal curvilinear coordinate systems a favourable ninepoint discretization is worked out which can be applied favourably e.g. to spherical mesh grids. The field calculation in magnetic deflection systems by means of an integral equation method is also highly advantageous. The methods for the field calculation can be still more improved by means of suitable hybrid procedures.

A second and shorter contribution is concerned with ray tracing and aberrations. Some favourable numerically stable new forms of the ray equation are derived and thereafter a new simple method for the determination of aberrations is outlined.

Key words: field calculation, ray tracing, aberrations, integral equation, hybrid method, Poisson's equation, discretization.

Introduction

Due to the rapid advances in computer technology it is possible to calculate now with reasonable effort and sufficient accuracy the properties of electron optical systems, and this is done very frequently, since the aid of a computer facilitates essentially the design of new devices. Generally such a computer-aided design consists of four subsequent and partly interdependent steps. These are the calculation of electric and magnetic fields from given source distributions and boundary conditions, the tracing of electron trajectories through these fields, the determination of paraxial properties and of aberrations from the obtained trajectories and finally the optimization of the design in question. The latter involves a repetition of the preceding steps under suitable variations of system parameters, until a relative minimum of the resulting aberration is found. In all of the above mentioned fields some progress was made during the last years, and it is the aim of this paper to present a short review of this progress and to give some outlook on further developments.

Field calculation

Generally three different methods of field calculation are in widespread use, these are the finite-element method (FEM), the finite-difference method (FDM) and the integral-equation method (IEM). Each of these has specific advantages and also disadvantages, so that none of them can be ignored completely or dealt with exclusively.

The finite-element method

The FEM consists in the dissection of the domain of solution into suitably chosen volume elements which must be irregular in the general case in order to fit to the boundaries. In the case of two-dimensional problems the mesh grid obtained in this way consists usually of irregular triangles with six elements joining together in each internal node.

It is familiar to derive the necessary equations for the values of the potential in the nodes from a variational principle: in each of the finite elements the stored electric or magnetic field energy must be minimized. In order to evaluate this principle, some assumptions about the required solution must be made. The simplest one is that the potential is a piecewise linear function. This version of the FEM has been introduced by Munro (1971, 1973) who applied it successfully to a large variety of electron optical devices, most recently to magnetic and electric deflection systems (Munro and Chu, 1982 a,b). A review of applications of Munro's method to the design of unconventional magnetic lenses is given by Mulvey (1982).

While the version of the FEM, described above is still frequently used, great improvements have been made in the past decade, mainly outside electron optics.Better approximations than piecewise linear functions for the potential are worked out (Silvester and Konrad, 1973), more generally curvilinear and even infinite elements are employed (Lencova and Lenc, 1982) and other than variational formulations are proposed. A review of recent improvements of the FEM is given in a volume edited by Chari and Silvester (1980). Even with respect to the still most familiar case of planar triangular grids progress was made, as Hermeline (1982) proposed a new and reliable method for the automatic generation of such grids under given boundary conditions and other constraints.

In spite of all these improvements the FEM has still severe disadvantages, the most serious one being the fact that the interpolation in irregular mesh grids is too complicated in order to ensure the continuity of the field strength and its derivatives along lines crossing orthogonally the mesh lines of the grid. This imposes strong restrictions on the ray tracing,as will be outlined in the "Ray Tracing and Aberrations" section.

The finite-difference method

In the applications of this method, the domain of solution is covered by a regular, usually square-shaped mesh grid. Most frequently this grid does not fit to the boundaries, so that many irregular nodes are to be considered. Theoretically it is no problem to derive discretization formulae for arbitrary irregular configurations, but in practice the consideration of many different irregular situations makes the method inconvenient. Nevertheless, the FDM has the advantage that - besides exceptional cases in electron guns - the grid is regular within the domain of the electron beam, so that the necessary calculation of the field-strength can be performed with sufficient accuracy.A review of these standard techniques has been given by Kasper (1982).

An interesting modification of the FDM has been proposed by Kang et al. (1981, 1983). In order to overcome the difficulties arising from the extreme differences of geometrical dimensions in electron guns with field emission cathodes, they proposed the use of an exponentially increasing spherical mesh grid which they named SCWIM (spherical coordinate with increasing mesh). Indeed, in this way a reasonable accuracy can be achieved. This method can be further generalized and improved, as will be outlined now.

We start from a general self-adjoint partial differential equation (PDE)

$$\frac{\partial}{\partial u}\left(p^2 v^\alpha \frac{\partial V}{\partial u}\right) + \frac{\partial}{\partial v}\left(p^2 v^\alpha \frac{\partial V}{\partial v}\right) + p^2 v^\alpha \left(\hat{q} V + s\right) = 0, \qquad (1)$$

p(u,v), q(u,v) and s(u,v) being non-singular analytic functions of the variables u and v, further $p > 0$, $\alpha \geq -1$, $v \geq 0$. The exponent α arises from a possible axial symmetry of the potential V(u,v), for instance $\alpha = 1$ for rotationally symmetric fields and $\alpha = 2m + 1$ for multipole fields of order m. The product-relation

$$V(u,v) = U(u,v)/p(u,v) \qquad (2)$$

reduces (1) to

$$\Delta_\alpha U = -g(u,v) := q(u,v)\cdot U - p \cdot s \qquad (3)$$

with

$$\Delta_\alpha := \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} + \frac{\alpha}{v}\cdot\frac{\partial}{\partial v} \qquad (4)$$

and

$$q(u,v) = \hat{q}(u,v) - p^{-1}\,\Delta_\alpha p \qquad (5)$$

For the discretization of (3) very accurate nine-point-formulae have been derived (Kasper, 1976), but with respect to the transformation (2) a still more favourable form of the discretization can be found. If we introduce the coordinates u = ih, v = kh (i,k integers) of the nodes and use corresponding subscripts ($U_{i,k} := U(ih, kh)$) then we can introduce favourably a new field

$$W_{i,k} := U_{i,k} + \frac{h^2}{12}\cdot g_{i,k} = p_{i,k}\left(V_{i,k} + \frac{h^2}{12}\left(q_{i,k} V_{i,k} + s_{i,k}\right)\right) \qquad (6)$$

and have now for $k \geq 1$:

$$W_{i,k} = A_{-1,k} W_{i,k-1} + A_{1,k} W_{i,k+1} + A_{0,k} h^2 g_{i,k} + \sum_{j=-1}^{1} B_{i,j}\left(W_{i-1,k+j} + W_{i+1,k+j}\right) + O(h^6) \qquad (7)$$

with the coefficients

$$\gamma_k := \frac{3\alpha(\alpha-2)}{10(24k^2+\alpha^2-2\alpha-6)},$$

$$A_{\pm1,k} = \frac{1}{5} \pm \frac{\alpha}{10k} + \gamma_k\left(1 \mp \frac{2\alpha+5}{6k}\right),$$

$$A_{0,k} = \frac{3}{10} - \gamma_k, \quad B_{0,k} = \frac{1}{5} - \gamma_k,$$

$$B_{\pm1,k} = \frac{1}{20} \pm \frac{\alpha}{40k} \mp \gamma_k \cdot \frac{\alpha+1}{12k}. \qquad (8)$$

On the axis of symmetry, that means for k = v = 0, instead of (7) and of (8) the formula

$$W_{i,0} = A_{1,0} W_{i,1} + \sum_{j=0}^{1} B_{j,0}(W_{i-1,j} + W_{i+1,j}) + h^2\left(A_{0,0}\, g_{0,0} + C(g_{0,0} - g_{0,1})\right) + O(h^6) \qquad (9)$$

with the coefficients

$$\beta := \frac{(1+\alpha)(6+\alpha)}{6(3+\alpha)}, \quad \gamma_0 := \frac{1}{2(2+\alpha-\beta)},$$

$$A_{0,0} = \gamma_0, \quad A_{1,0} = 2\gamma_0(1+\alpha-\beta),$$

$$B_{0,0} = \gamma_0(1-\beta), \quad B_{1,0} = \gamma_0\beta,$$

$$C = \gamma_0 \frac{\alpha(1+\alpha)}{6(3+\alpha)}. \qquad (10)$$

is to be employed. The derivation of this discretization cannot be presented here and will be published elsewhere.

A good example for the practical application of these formulae is the SCWIM grid. This can be considered as a conformal mapping of an originally cylindric grid with square-shaped meshes in the axial section. Let (z,r,ϕ) denote cylindric coordinates and (R,Θ,ϕ) coaxial spherical coordinates with $z = R\cos\Theta$, $r = R\sin\Theta$, then we have

$$z + ir = R\exp(i\Theta) = R_0\exp(u+iv) \qquad (11)$$

with $R = R_0\exp(u)$ and $v \equiv \Theta$. Transforming the rotationally symmetric Poisson equation $\nabla^2 V = -\varepsilon_0^{-1}\rho(R,\Theta)$ into these coordinates, we find

$$\frac{\partial}{\partial u}\left(e^u \sin v \frac{\partial V}{\partial u}\right) + \frac{\partial}{\partial v}\left(e^u \sin v \frac{\partial V}{\partial v}\right) = \varepsilon_0^{-1} R_0^2 e^{3u} \sin v \cdot \rho(R_0 e^u, v). \qquad (12)$$

This can be cast into the form (1) with

$$\alpha = 1, \quad p^2 = e^u \frac{\sin v}{v}, \quad \hat{q} = 0, \quad (v < \pi),$$

$$s = \varepsilon_0^{-1} R_0^2 e^{2u} \cdot \rho(R_0 e^u, v),$$

$$q = \frac{1}{4}\left(\frac{1}{\sin^2 v} - \frac{1}{v^2}\right) = \frac{1}{12}\left(1 + \frac{v^2}{5}\right) + O(v^4). \qquad (13)$$

On the optical axis the coefficients p and q remain positive. By virtue of (11) the SCWIM-grid is transformed into an ordinary square shaped grid in u and v. The discretization error is now of sixth order in the mesh width. Numerical tests have shown that in comparison with a five-point-discretization with the same mesh width a decrease of the error by a factor 10^{-5} can be achieved (Killes, to be published). But this is true only in the case of regular grids. Irregular meshes in the vicinity of boundaries will cause complications and a loss of accuracy. This can be circumvented by a combination of the FDM with the IEM, as will be obvious further below.

The integral-equation method

In the case of pure surface charge distributions with density $\sigma(\underline{r})$ the electrostatic potential satisfies

$$V(\underline{r}) = \int_B \frac{\sigma(\underline{r}')\, d^2r'}{4\pi\varepsilon_0 |\underline{r} - \underline{r}'|}, \qquad (14)$$

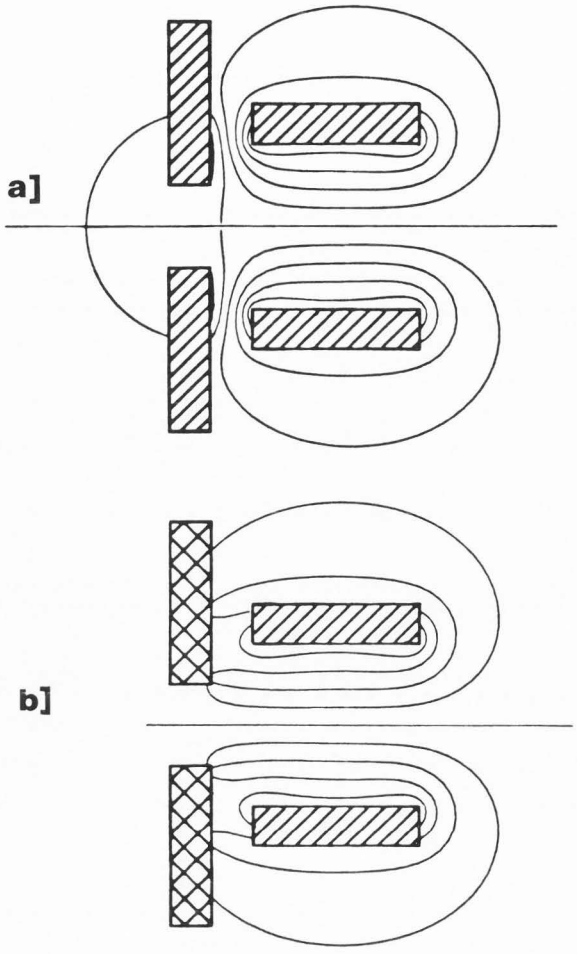
where the integration is to be carried out over the boundary B. In the case of Dirichlet problems the boundary values of $V(\underline{r})$ are prescribed and (14) is then an integral equation for the unknown source distribution $\sigma(\underline{r})$. After its solution, (1) can be used in order to determine $V(\underline{r})$ in an arbitrary point $\underline{r}$. By means of an analogy-transfer also the magnetic field between unsaturated poles with very high permeability can be calculated. This version of the IEM, called the surface-charge method (SCM), is quite familiar in electron optics.

In order to perform the required integration, some simplifications are necessary. It is customary to dissect the surface into a large number of sufficiently small area elements in which $\sigma(\underline{r})$ can be considered as practically constant, then the integration can be carried out analytically and (14) is replaced by a linear system of equations for the piecewise constant, but unknown values of σ. The numerous publications concerning this matter differ only in details of the necessary discretization. Instead of discussing these items, we consider some recent developments.

Scherle (1983a) has applied the IEM to the calculation of magnetic fields in shielded deflection systems with toroidal and saddle coils, respectively. He was able to take into account the finite permeabilities of core materials and to solve the corresponding interface-condition problems. Hence his version of the IEM is far more general than the SCM outlined above. The starting point is the familiar separation of the magnetic field into the pure contribution $\underline{H}_0(\underline{r})$ from the coils, satisfying

$$\operatorname{div} \underline{H}_0(\underline{r}) = 0, \quad \operatorname{curl} \underline{H}_0(\underline{r}) = \underline{j}(\underline{r}) \qquad (15)$$

and hence determined from the theorem of Biot and Savart, and a gradient field $\operatorname{grad} V(\underline{r})$ generated by the ferrite cores:



Figures 1a,b: equipotentials of the scalar magnetic pseudo-potential $V(\underline{r})$ in an axial section through a system of saddle coils, a ferromagnetic core and a shielding plate with a bore. For reasons of clearness the coils and their field $\underline{H}_0(\underline{r})$ are omitted.
(a) ferromagnetic shielding plate
(b) superconducting shielding plate
Courtesy of W. Scherle (1983b).

$$\underline{H}(\underline{r}) = \underline{H}_0(\underline{r}) + \text{grad } V(\underline{r}) \qquad (16)$$

The latter contribution has its sources on the core surfaces and satisfies a Fredholm equation of second kind:

$$\frac{\mu+\mu_0}{2(\mu-\mu_0)} V(\underline{r}) + \int_B V(\underline{r}') \frac{\partial}{\partial n'} G(\underline{r},\underline{r}')\, d^2r' = -\int_B G(\underline{r},\underline{r}')\, \underline{n}' \cdot \underline{H}_0(\underline{r}')\, d^2r', \qquad (17)$$

$\underline{n}'$ being the local surface normal in the directon towards the vacuum and $G = (4\pi|\underline{r}-\underline{r}'|)^{-1}$ Green's function of free space.

In the case of rotationally symmetric cores, even for unround current distributions $\underline{j}(\underline{r})$, eq.(17) can be reduced to a sequence of uncoupled one-dimensional Fredholm equations of second kind, as each term in (17) is expanded into a Fourier series with respect to the azimuth round the optic axis. After the decouplings, obtained in this way and the analytic integration over the azimuth, the remaining integration runs over the length s' of arc in the meridional section C through the boundaries. The resulting equations to be solved have the principal structure

$$\int_C K(s,s')\, y(s')\, ds' = U(s) + \lambda y(s), \qquad (18)$$

U(s) being a given boundary value function, y(s) the required function, λ a fixed constant and K(s,s') a complicated kernel function with logarithmic singularity at s = s'.

Scherle (1983a) has used a cubic spline function for y(s) and in this way he obtained a high accuracy for y(s). In his thesis (1983b) he has developed a still more general version of the IEM for two different cores. The items cannot be described here, the plots of potentials, calculated in this way, are presented in fig. 1a,b.

In order to facilitate the integration over logarithmic singularities, Kasper (1983) has derived a new integration formula for functions with logarithmic singularities. This can be further generalized. Let $f_i(x)$, i = 1,2,3 be arbitrary regular functions, then we have

$$F(x) := f_1(x)\, \ln|x| + f_2(x)/x + f_3(x),$$

$$\int_{-h}^{h} F(x)\, dx = h \sum_{\mu=1}^{4} G_\mu \left(F(p_\mu h) + F(-p_\mu h) \right) + O(h^9) \qquad (19)$$

with the abscissas and weight factors given by Basche (private communication, to be published)

$P_1 = 0.0399\ 4596\ 2203$
$P_2 = 0.2801\ 7249\ 6204$
$P_3 = 0.6361\ 2394\ 4954$
$P_4 = 0.9223\ 6045\ 1138$

$G_1 = 0.1270\ 7679\ 2574$
$G_2 = 0.3267\ 4117\ 6078$
$G_3 = 0.3523\ 4912\ 8452$
$G_4 = 0.1938\ 3290\ 2896$

The function y(s) was originally represented by a quadratic spline, i.e. a piecewise quadratic function with a continuous first derivative, in order to make eq. (19) applicable to the integration in eq. (18). This gives already highly accurate results. The details shall not be explained here. Instead of doing this, we present a still more improved method which can be found with very little effort.

We dissect the integration contour C into suitably chosen intervals, $s_0 < s_1 < s_2 \cdots < s_N$ and choose an expansion in terms of Legendre polynomials,

$$y(s) = \sum_{\ell=0}^{M} c_i^{(\ell)} P_\ell(t) \quad , \quad s_{i-1} \le s \le s_i \qquad (20)$$

with

$$h_i := (s_i - s_{i-1})/2 \quad , \quad \sigma_i := (s_i + s_{i-1})/2$$
$$t := (s - \sigma_i)/h_i \quad , \quad i = 1....N \qquad (21)$$

Introducing the matrix elements

$$M_{i,k}^{(\ell)} = h_k \int_{-1}^{1} K(\sigma_i, \sigma_k + t h_k) P_\ell(t)\, dt - \lambda P_\ell(0)\, \delta_{i,k} \quad , \quad (i,k = 1 \cdots N) \qquad (22)$$

and the source terms $U_i := U(\sigma_i)$ we obtain the linear system of equations

$$\sum_{\ell=0}^{M} \sum_{k=1}^{N} M_{i,k}^{(\ell)} c_k^{(\ell)} = U_i \quad , \quad i = 1 \cdots N. \qquad (23)$$

Provided that the coefficients $c_k^{(\ell)}$ for $l \neq 0$ are known, we can solve this for $c_1^{(0)} \ldots c_N^{(0)}$. By these coefficients the integral over the solution y(s) is determined: With the definition

$$Y(s) := \int_{s_0}^{s} y(s')ds' \quad , \quad Y_i := Y(s_i) \qquad (24)$$

we have $Y_0 = 0$ and

$$Y_i = Y_{i-1} + 2h_i c_i^{(0)} \quad , \quad i = 1...N \; . \qquad (25)$$

Now we can determine $y_1 \ldots y_N$ and $y_1' \ldots y_N'$ by means of numeric differentiation. With these we obtain linear equations for the coefficients $c_i^{(\ell)}$ with $i = 1....N$ and $1 \le l \le M = 4$:

$$c_i^{(1)} = (6(y_i - y_{i-1}) + h_i(y_i' + y_{i-1}'))/10$$
$$c_i^{(3)} = (-(y_i - y_{i-1}) + h_i(y_i' + y_{i-1}'))/10$$
$$c_i^{(2)} = (10(y_i + y_{i-1} - 2c_i^{(0)}) - h_i(y_i' - y_{i-1}'))/14$$
$$c_i^{(4)} = (-3(y_i + y_{i-1} - 2c_i^{(0)}) + h_i(y_i' - y_{i-1}'))/14 \qquad (26)$$

These are again substituted into (23). Starting with $c_k^{(\ell)} = 0$ for $l \neq 0$ in the first loop, the whole system of relations can be solved iteratively and converges rapidly. The accuracy is high if the function U(s) varies slowly. A modification for more rapidly varying functions U(s) is being investigated. Details will follow in a separate publication. In summary this method can be made highly accurate and efficient.

For truly three-dimensional problems the general situation is less favourable. It is not only the enlarged number of dimensions which causes problems, but - more than this - the fact that it is often impossible to map the given surfaces in a regular mesh grid in a two-dimensional parametric space. Concerning the surfaces there may arise similar difficulties like those in the FEM. A practicable approximation for the solution of Dirichlet problems in three dimensions has been published by Eupper (1982) who replaced the surface charge distribution by a set of suitably charged bars located behind the electrode surfaces. The charge distribution on these bars is determined in such a way that the potential assumes its prescribed boundary values at a sequence of control points on the electrode surfaces. The results for a field emission cathode with the shape of a hipped roof are presented in figs 2a,b.

Combinations of methods

In many practical cases a suitable combination of different field calculation methods can be more advantageous than the use of only one pure method. With respect to Dirichlet problems this question has been investigated in details by Schaefer (1982, 1983). His theory shall not be outlined here, since it is described in a separate paper at this conference (see Schaefer, this volume).

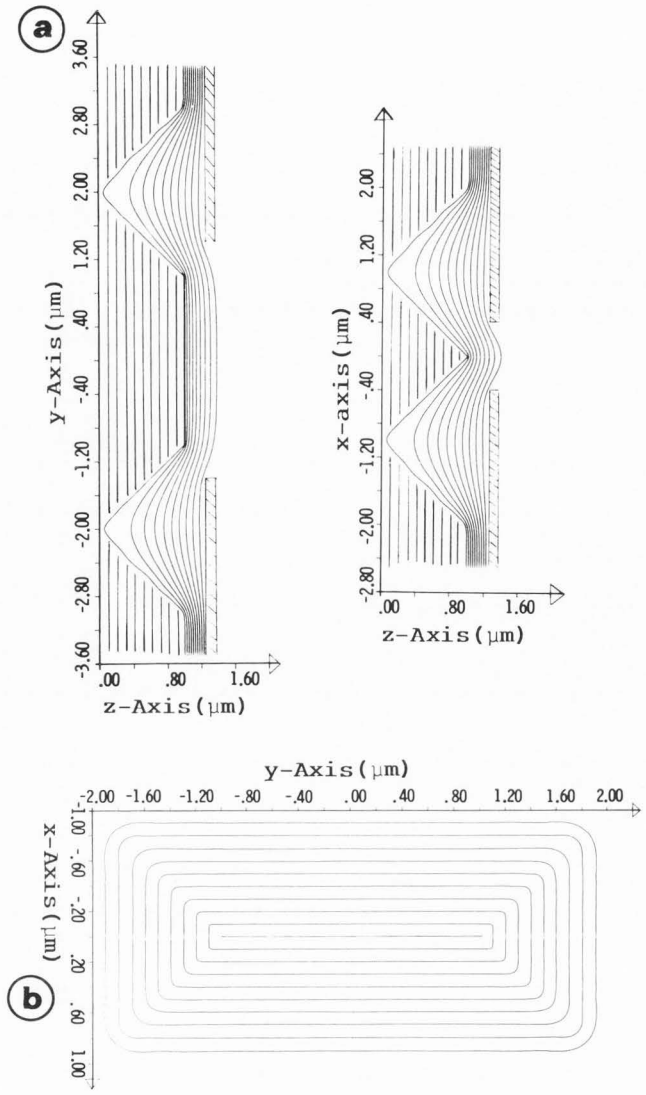
In this paper we shall consider first a combination between the IEM and the FDM, which is shown in fig. 3. We want to solve a Dirichlet problem for a domain G with boundary ∂G:

$$\nabla^2 V(\underline{r}) = -\varrho(\underline{r})/\varepsilon_0 \quad , \quad \underline{r} \in G \, , \qquad (27)$$

$$V(\underline{r}) = \bar{V}(\underline{r}) \quad , \quad \underline{r} \in \partial G \, . \qquad (28)$$

The IEM is very favourable for the solution of Laplace's equation, even in the case of complicated boundaries, but is unsuitable for Poisson's equation, since the numerical evaluation of Coulomb integrals is a very time-consuming procedure. On the other hand the FDM is a very fast method for the solution of Poisson's equation, but useful only in the case of simple boundaries.

In this situation we propose to extend the regular mesh grid beyond the boundary ∂G and to extrapolate the space charge distribution continuously up to the new boundary $\partial \tilde{G}$. On $\partial \tilde{G}$ now simple guessed boundary values for a potential W are assumed and the PDE $\nabla^2 W = -\varrho/\varepsilon_0$ is solved using the FDM. On ∂G we find then, of course, wrong boundary values $\bar{W}(\underline{r})$, but this is no misfortune. The true solution V can differ from the particular one (W) only by an appropriate solution U of Laplace's equation $\nabla^2 U = 0$. Hence we have to solve now



Figures 2a,b: equipotentials in different sections through a field electron emission source consisting of a cathode with a hipped roof and an anode with a rectangular bore.
Courtesy of M. Eupper (1982)

$$\nabla^2 U(\underline{r}) = 0 \quad , \qquad \underline{r} \in G \tag{29}$$

$$U(\underline{r}) = \bar{V}(\underline{r}) - \bar{W}(\underline{r}) \quad , \qquad \underline{r} \in \partial G \tag{30}$$

by means of the IEM in order to find $V = U + W$ as the correct total solution. In this way we have combined the advantages of both methods and circumvented their disadvantages.

This hybrid method shall be applied to the field calculation in electron guns with space charges, where it seems to be most useful; a corresponding publication is in preparation. In this context it is to be mentioned that the method outlined above is only one of the many possibilities to combine different procedures. For instance, in the vicinity of a spherical cathode, both the space charge distribution $\varrho(\underline{r})$ and the particular potential $W(\underline{r})$ can be expanded in series expansions containing Legendre polynomials, e.g.

$$W(R,\Theta) = \frac{1}{R} \sum_{l=0}^{L} \phi_l(R) P_l(\cos\Theta) \tag{31}$$

For the coefficient functions $\phi_l(R)$ a sequence of simple decoupled ordinary differential equations can be derived which are easily solved numerically. This procedure has been worked out by Weysser (1983a,b), who treated in this way an electron gun with a hemispherical tip cathode (fig. 4).

Finally we consider a simple combination between the FEM and the IEM, suitable for the field calculation in round magnetic lenses with saturation, as is shown in fig. 5. The FEM is advantageous for the field computation in nonlinear media, hence we discretize the axial section through the pole by a suitable triangular grid. Then using the FEM, we can calculate the values of the azimuthal vector potential $A(z,r)$ at the internal nodes, provided that the boundary values at the pole surfaces are known. Usually the latter are determined by the FEM in a grid extended to the practically field free space. This is, however, unfavourable; instead of this we better apply the IEM to the vacuum part of the field; then we have to solve the integral equation

$$\frac{1}{2}A(z,r) = \oint \left[A(z',r')\,\partial G_1/\partial n' - G_1(z,r;z',r')\left(\partial A(z',r')/\partial n'\right)_v \right] r'\,ds' + \mu_0 \iint G_1(z,r;z',r')\, j(z',r')\, r'\,dr'\,dz' \tag{32}$$

for the potential distribution on the pole surface. Here ds' denotes the length element of arc, j(z,r) the azimuthal current density in the coils and $\partial/\partial n'$ the normal derivative in the direction towards the vacuum and on the vacuum side of the surface. The corresponding Green function is given by:

$$G_1(z,r;z',r') = \frac{1}{4\pi} \int_0^{2\pi} \frac{\cos\alpha \; d\alpha}{\sqrt{(z-z')^2 + r^2 + r'^2 - 2rr'\cos\alpha}} \tag{33}$$

This is an elliptic integral which can be calculated by well-known procedures. It has a logarithmic singularity, hence even the integration over the normal derivative by means of (19) is straightforward.

The solution of (32) requires the knowledge of $(\partial A/\partial n)_v$ on the vacuum side of the boundary. This derivative can be obtained in the following way. The FEM

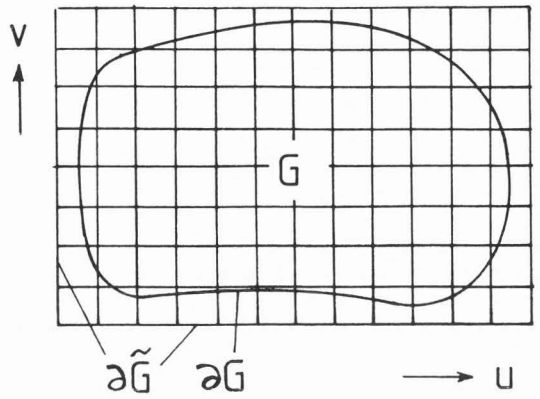


Figure 3: extension of a regular mesh grid beyond the curved boundary ∂G of a given domain G.

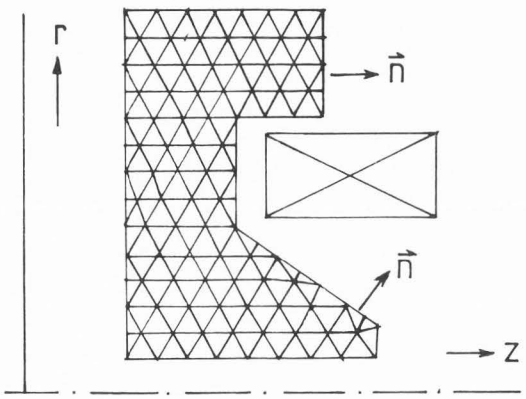


Figure 5: half axial section through an open round magnetic lens with a ferromagnetic core and a rectangular distribution of windings. Only the interior of the core is discretized by a triangular mesh grid.

can be formulated in such a manner that in each element the field strength $\underline{B}$ is calculated by means of numerical differentiation. Hence we know then $(\partial A/\partial n)_i$ on the inner side of the boundary. Moreover we can determine the reciprocal permeability by differentiation of the functional for the stored magnetic energy with respect to $B = |\underline{B}|$. But then $(\partial A/\partial n)_v$ is determined by the continuity of the tangential H-component:

$$\mu^{-1}\left[\partial(rA)/\partial n\right]_i = \mu_0^{-1}\left[\partial(rA)/\partial n\right]_v .$$

The whole system of equations has to be solved iteratively. This is no disadvantage, since for solving nonlinear problems iterative techniques are unavoidable in any case. Eventually the evaluation of $(\partial A/\partial n)_v$ requires an under-relaxation

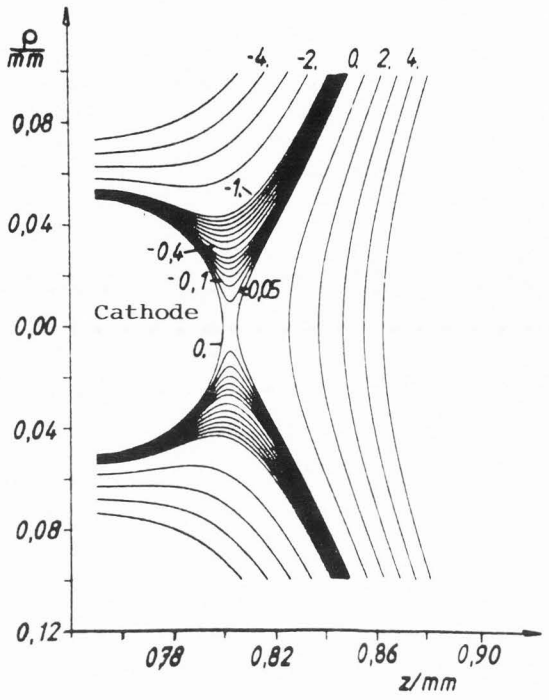


Figure 4: equipotentials in the vicinity of a hemispherical cathode. Due to the influence of space charge the potential is negative in front of the cathode. The cathode shank following to the left hand side, is not shown in this figure. Courtesy of R. Weysser (1983b)

for reasons of stability; but this provides no principal problem. The computing time can be kept reasonably short, since the time-consuming calculation of the matrix elements for the solution of the integral equations needs to be carried out only once in the first loop. The practical investigations concerning this method are still going on and will be published later.

This technique removes the main disadvantage of the FEM, i.e. the inaccurate interpolations and differentiations in the vacuum part of the field. The essential gain is that now the field strength is truly a smooth analytic solution of the field equations with a relative error of about 10^{-3} or less. Then the ray tracing, especially for sufficiently large distances from the pole surfaces, provides no longer any problem.

Ray tracing and aberrations

The possibility and the quality of ray tracings depend strongly on the accuracy of the field calculation. If only the axial electrostatic potential $\phi(z)$, the axial flux density B(z) or other axial functions are computed by use of

the FEM, then only the paraxial ray equations can be solved and this imposes the strong restriction to deal exclusively with the standard perturbation theory of aberrations. Probably this is the reason why the latter theory has been worked out in many details.

The physics of round magnetic lenses is developed in very many details and presented comprehensively in a volume edited by Hawkes (1982). Another comprehensive presentation of the aberration theory, also given by Hawkes (1980), deals with more general systems. Many items can also be found in the conference proceedings edited by Wollnik (1981). Here the quite numerous citations, to be found in these publications, shall not be repeated again. Some recent papers, not yet cited in the references given above, concern the aberration theory for microwave cavity lenses (Hawkes 1982/83 and 1983), for general systems with parasitic errors (Plies 1982a,b) and for planar cathode lenses (Ximen Ji-ye et al., 1983).

A quite general feature of the perturbation theory is its enormous complexity which forces many authors to use the aid of computer algebra languages; for instance, Hawkes applied the language CAMAL and Soma (1977) the language REDUCE. Usually the aberration coefficients are represented as integral expressions which assume such a length, that an outsider may have difficulties with them. Moreover, there are systems for which an aberration theory of third order is insufficient; examples are electrostatic filter lenses (Niemitz, 1980), deflection units at large deflection angles and annular systems like beta spectrometers of Siegbahn's type. Hence new concepts seem to be necessary.

Some ray equations

The accurate calculation of electron trajectories does not make any problem, provided that the electromagnetic fields can be computed accurately at arbitrary points of reference. Hence the effort is to be concentrated on the improvement of the field calculation programs. When this has been achieved, practically every kind of ray equation can be solved numerically. In Tuebingen we have good experience with a parametrization of the Lorentz equation in terms of a variable σ proportional to the relativistic proper time:

$$\ddot{\underline{r}}(\sigma) = \nabla\varphi(\underline{r}) + \underline{b}(\underline{r}) \times \dot{\underline{r}}(\sigma) \qquad (34)$$

Here dots denote differentiations with respect to σ, further

$$\varphi(\underline{r}) = \phi^*(\underline{r})/(2U^*) \qquad (35)$$

is a normalized relativistic acceleration potential and

$$\underline{b}(\underline{r}) = \sqrt{\frac{e}{2m_0 U^*}}\ \underline{B}(\underline{r}) \qquad (36)$$

a normalized magnetic field strength. The choice of the normalization constant U^* is free; very suitable is often the asymptotic acceleration potential $U^* = \phi^*(\infty)$.

The solution of (34) must satisfy the conservation law

$$\dot{\underline{r}}^2 = 2\varphi(\underline{r}) + \text{const}\ , \qquad (37)$$

the constant being determined uniquely by the bias of the electric potential and by the kinetic starting energy. The ray equation (34) is suitable for all systems with time-independent fields. Besides this applicability in numerical procedures, the particular choice of the parameter σ has the advantage that (34) is the simplest possible form of the general relativistic ray equation. This is the basis of the subsequent considerations.

Sometimes it is favourable to solve the ray equation not in the given form but in an incremental form yielding directly the shift $\underline{s}(\sigma)$ relative to another trajectory $\underline{r}(\sigma)$. The latter may be, for instance, the optical axis in a magnetic deflection prism. Small differences between neighbouring values of an arbitrary smooth function $f(\underline{r})$ can be avoided by numerical integration over its gradient:

$$\begin{aligned} f(\underline{r}) :&= f(\underline{r} + \underline{s}) - f(\underline{r}) \\ &= \underline{s} \cdot \int_0^1 \nabla f(\underline{r} + t\underline{s})\, dt. \end{aligned} \qquad (38)$$

This integration can be performed e.g. by means of Gauss quadrature formulae and gives always a reliable result, regardless how small $|\underline{s}|$ may be. In this sense we obtain from (34) quite correctly

$$\begin{aligned} \ddot{\underline{s}}(\sigma) = &\Delta\,(\nabla\varphi(\underline{r})) + \underline{b}(\underline{r}) \times \dot{\underline{s}} \\ &+ \Delta\,\underline{b}(\underline{r}) \times (\dot{\underline{r}} + \dot{\underline{s}})\ . \end{aligned} \qquad (39)$$

This is valid for electrons having the same total energy. This ray equation can be generalized easily in order to include chromatic aberrations. The experiences made with (39) are still in the beginning; they will be published in a later paper.

Evaluation of aberration discs

By a solution of (34) and of (39) it is possible to determine accurately the endpoints of electron trajectories in a given recording plane, the initial conditions being still quite general. If we compute trajectories starting in one common object point with directions located on an aperture cone, the line connecting the obtained endpoints forms the contour of the corresponding aberration disc.This

can be repeated for different aperture angles. A typical example is given in figs. 6a and 6b, which have been determined by Killes (1983, unpublished). These figures are the aberration discs for an axial object point in a double focusing magnetic sector field spectrometer. The effect of a small defocus is quite obvious. These contours have been obtained by a numerical solution of (34), numerical instabilities are not to be noticed.

A quite simple and practicable method for the quantitative evaluation of aberration discs has been developed by Scherle (1983). Let (x_k, y_k) denote the coordinates of individual trajectories in a given recording plane z = const, (x'_k, y'_k) the corresponding slopes and g_k suitable positive weight factors normalized to unit sum. Then

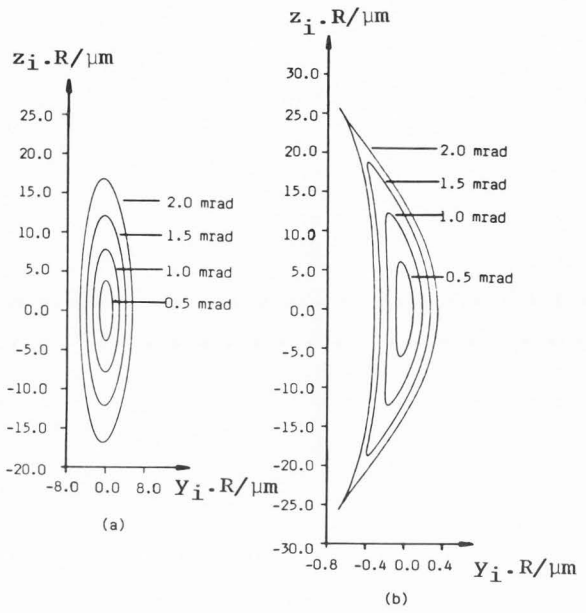
$$\bar{x} = \sum_{k=1}^{N} g_k x_k, \quad \bar{y} = \sum_{k=1}^{N} g_k y_k \tag{40}$$

are the coordinates of the center of the aberration disc; their deviations from the Gaussian image coordinates can be interpreted as weighted distortions. Furthermore, the second moments of the aberration disc are defined by

$$\begin{aligned} S_{xx} &= \sum g_k (x_k - \bar{x})^2, \\ S_{xy} &= \sum g_k (x_k - \bar{x})(y_k - \bar{y}), \\ S_{yy} &= \sum g_k (y_k - \bar{y})^2. \end{aligned} \tag{41}$$

By these a variance ellipse is defined which approximates the cross section of the beam. A good approximation is obtained in many practical cases if the semiaxes of the ellipse are enlarged by a factor 2. Since the slopes of the trajectories are known, the local tangents are given. Hence, as far as it is sufficient to approximate the true trajectories by their tangents, for instance in a field free image space, the determination of the ellipse can be repeated for any plane z = const. In this way a defocus can be studied quite easily and rapidly. Fig. 7 demonstrates the approximation found for the spherical aberration of a round lens. The approximate circle of minimum radius is located near the familiar circle of least confusion.

Though this procedure is clearly an approximate one, it is certainly more convincing than the familiar practice to calculate a root-mean-square radius from roughly guessed radii for different aberration terms. If ever necessary, Scherle's theory can be further improved by taking into account the moments of third or higher order. It has one advantage which may be useful in the future: obviously the aberrations are minimized if after



Figures 6a,b: examples for contour lines of aberration discs in a double focusing magnetic sector field with 90 degrees-deflection perpendicular to the z-direction. The rays start in an axial object point, the initial slopes form cones with the given semiaperture angles.
(a) configuration close to the best obtained focus
(b) defocus of 3 mm for a deflection radius 25 cm
Courtesy of P. Killes (unpublished work)

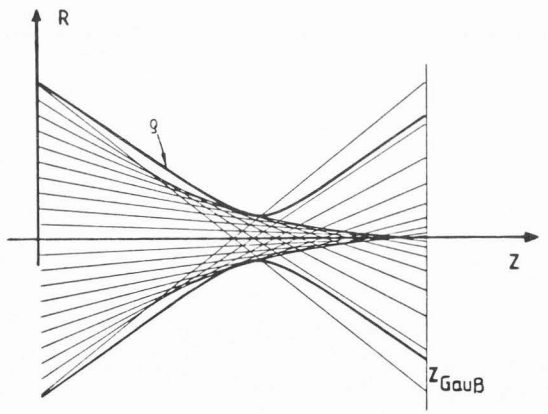


Figure 7: Scherle's approximation of the spherical aberration in a conventional round lens (the slopes are enlarged for reasons of distinctness). The hyperbola marked by ϱ represents the approximation. Courtesy of W. Scherle (1983b)

all allowed variations of system parameters the maximum diameter of all aberration discs has its smallest possible value. This gives a clear concept for optimization procedures. The practical application of this idea is still in the beginning, but seems to be straightforward.

In the case that not only the information about entire aberration discs is needed but also the knowledge of aberration coefficients, the latter are to be determined by suitable least-squares-fits with the endpoints (x_k, y_k), (k = 1...N) of numerically calculated trajectories. Since this requires a very high accuracy, some care must be taken in the set-up of the corresponding routine. Such calculations were, for instance, performed by Niemitz (1980), who determined in this way the aberration coefficients for electrostatic filter lenses, even in fifth and higher orders. The research concerning the improvement of least-squares-fit techniques is going on. In summary there are already now some alternatives to the standard perturbation theory of aberrations.

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