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Charged particle optics : Principles and applications

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What is geometrical optics? What is an image?









Fermat and the principle of least time : a « causa sive ratio » for the refraction INSA (cnrs TOULOUSE

• Pierre de Fermat (1601-m. 1665)

« Synthèse pour les réfractions » (1662)

« Je reconnais premièrement avec vous la vérité de ce principe, que la nature agit toujours par les voies les plus courtes. Vous en déduisez très bien l'égalité des angles de réflexion et d'incidence »











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The idea behind the concept of Hamilton's characteristic function



$$\delta L = \delta \int_{P_1}^{P_2} n(x, y, z) ds = 0$$



$$L = \int_{A}^{B} \left(n(x, y, z) \sqrt{1 + x^{2} + y^{2}} \right) dz$$





Principle of optics

Foundations of geometrical optics (introduction) : Eikonal functions and aberration series

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In optics time is the function that must be minimized. Linked to the optical path length L given by :

 $L = n_1 d_1 + n_2 d_2 + n_3 d_3 + \dots$

https://phet.colorado.edu/sims/html/bending-light/latest/bending-light_all.html?locale=es

→ What is geometrical optics? How do we make high-performance instruments?



Fermat's principle : consequences

















Johann Carl Friedrich Gauß (1777-m. 1855)

« Dioptrische Untersuchungen (1856) »





Definition of the stigmatic imaging condition: linear approximation of the optical length



Axe optique Paraxial





Geometrically a **perfect imaging process** is defined by :

The optical length any curve in the object space is equal to the optical length of it's image It corresponds to a *linear transformation*

 $L_A = L_A^{(0)} + L_A^{(2)}$



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\mathbf{N} Description of the optical system under the paraxial approximation : the cardinal planes \mathbf{crrs}

- ► *P* : principal planes
- S : intersection surfaces/optical axis
- F : focal planes
- f: focal distances
- r : radii of curvature of surfaces
- d : thickness SS'
- \bullet *n* : refraction index





Description of the optical system under the paraxial approximation : the fundamental rays

- The principal ray defines the maximum field. Intersection with optic axis : defines the pupil planes



between marginal (aperture) and principal (field) rays :

$$u(z) = \alpha h(z) + yg(z)$$

The marginal ray defines the maximum aperture angle. Intersection with optic axis : defines the Gaussian image planes

 \rightarrow Under paraxial approximation, any ray (define by it's angle α and field height y) can be written using linear combination.







Mathematical optics and the design of high-performance instruments

Karl Siegmund Schwarzschild (1873-m. 1916)

« Untersuchungen zur geometrischen (1905) »



Developed a Hamiltonian approach to the calculation of Seidel aberrations. He builds on Bruns' work and develops his own characteristic function (or eikonal).

• Heinrich Bruns (1848-m. 1919) « Das Eikonal (1895) »



 $-2R_{\circ}\varrho_{1}H^{2}h^{9}\left\{\frac{b}{r^{3}}+\frac{K(2L-K)}{r}\right\}$ $+4R_{o}\varkappa_{o1}H^{3}h\left\{\frac{b}{r^{3}}+\frac{L(2L-K)}{r}\right\}$ $+ 4\varrho_1 \varkappa_{o_1} H h^{s} \bigg\{ \frac{b}{r^3} + \frac{KL}{r} \bigg\}.$ Wir gehen sofort weiter und bilden:

 $-\varrho_1^2 h_4 \left\{ \frac{b}{r^3} + \frac{K^2}{r} \right\}$

 $-4\varkappa_{01}^{2}H^{2}h^{2}\left\{\frac{b}{r^{3}}+\frac{L^{4}}{r}\right\}$

4. Die Fehler eines beliebigen Spiegelsystems. Nach dem I. § 5 abgeleiteten Satze ergeben sich dieselben durch Superposition der fehler der Einzelsysteme, welche durch die Entwicklungskoeffizienten des eben efundenen Eikonals dargestellt werden. Unterscheidet man die verschiedenen intereinander gesetzten Spiegel durch Indices i = 1 bis i = k, so findet man völliger Analogie zu I. § 6 (54):

$$B = \sum_{i=1}^{k} h_{i}^{i} \left\{ \frac{b_{i}}{r_{i}^{3}} + \frac{K_{i}^{2}}{r_{i}} \right\}$$

$$C = \sum_{i=1}^{k} h_{i}^{2} H_{i}^{2} \left\{ \frac{b_{i}}{r_{i}^{3}} + \frac{L_{i}^{2}}{r_{i}} \right\}$$

$$D = \sum_{i=1}^{k} h_{i}^{2} H_{i}^{2} \left\{ \frac{b_{i}}{r_{i}^{3}} + \frac{K_{i}(2L_{i} - K_{i})}{r_{i}} \right\}$$

$$E = \sum_{i=1}^{k} h_{i} H_{i}^{3} \left\{ \frac{b_{i}}{r_{i}^{3}} + \frac{L_{i}(2L_{i} - K_{i})}{r_{i}} \right\}$$

$$F = \sum_{i=1}^{k} h_{i}^{2} H_{i} \left\{ \frac{b_{i}}{r_{i}^{3}} + \frac{K_{i}L_{i}}{r_{i}} \right\}.$$





Philipp Ludwig von Seidel (1821-m. 1896)

« Über die Entwicklung der Glieder 3ter Ordnung welche den Weg eines ausserhalb der Ebene der Axe gelegene Lichtstrahles durch ein System brechender Medien bestimmen (1856) »



ASTRONOMISCHE NACHRICHTEN. № 1027.

Zur Dioptrik.

Ueber die Entwicklung der Glieder 3ter Ordnung, welche den Weg eines ausserhalb der Ebene der Axe gelegenen Lichtstrahles durch ein System brechender Medien bestimmen, von Herrn Dr. L. Seidel.

Perturbations of Gaussian optics : 5 primary geometrical aberrations L^4 and 2 chromatics $L^2(\lambda)$













$$\Delta y' = -\frac{1}{n'} \frac{\partial L_A^{(4)}}{\partial s_v'}$$

$$S_x^4 + Bs_y^4 + Cs_x^2s_y^2 + Ds_x^2s_y^2 + \dots$$

$$(\theta) + Pr_p^2 y^2 + Ay^2 r_p^2 cos^2(\theta) + Dy^4$$

$$(L_A^{(4)})_{ptz} \quad (L_A^{(4)})_{astg} \quad (L_A^{(4)})_{dist}$$









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 \Rightarrow Representation using a 2-dimensional Taylor series expansion: field of view y and aperture angle u_y or pupil plane coordinate (r, θ)

The sum of the exponents must be constant according to the order of the aberration considered

			Spherical	Coma
Aper- ture r			y ⁰	y ¹
	Distortion	r ⁰		y cosθ Tilt
		r ¹	r ¹ Defocus	
		r²		y r²cos θ Coma primary
		r ³	r ³ Spherical primary	
		r ⁴		yr ⁴ cosθ Coma secondary
		r ⁵	r ⁵ Spherical secondary	

Aberrations series expansion







Going back to the quasi-real situation (paraxial + Seidel aberrations) ... INSA





⊕ Taper ici pour rechercher





 $y' = y_{para} + \Delta y' = -\frac{1}{n'} \frac{\partial L_A}{\partial s'_v}$















Wavefront aberrations W = differences between radius of Principal ray wavefront and the real wavefront in the pupil plane :

$$W = L_{P'Q'} = L_{OQ'} - L_{OP'} \approx L_A - L_A^{(2)} = L_A^{(4)}$$

Transverse aberrations $\Delta y'$ are then simply derived from wavefront aberration by differentiate it relatively to pupil coordinate (i.e. the aperture angles)

$$\Delta y' = -$$



(radius R = optical length of the principal ray)

$$R \cdot \frac{\partial W(x_p, y_p)}{\partial y_p}$$







Seidel primary aberrations : wavefront vs transverse aberrations



A. Spherical aberration B.Coma C.Astigmatism D.Petzval curvature E.Distorsion

Symmetry with respect to **Periodicity** ...





Mathematical optics and the design of high-performance instruments

Ernst Karl Abbe (1840-m. 1905)

« Beiträge zur Theorie des Mikroskops und der mikroskopischen Wahrnehmung (1873) »





Resolution limit for optical instruments







Carl Friedrich Zeiss (1816-m. 1888) « Zeiss company » : collaboration with Abbe



Zeiss microscope (1879) with Abbe optics



New illumination system developed by Abbe







After a while, the points on the object are no longer points in the image ...





Why ? And how does this affect the resolution?







Introduction to Variational mechanics

General history, introduction to main concepts and application to charged particles in static electromagnetic fields

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William Rowan Hamilton

(Dublin University Review and Quarterly Magazine, 1 (1833), pp. 795–826.)









Newtonian, Lagrangian and Hamiltonian approaches to physics

➡ What is the best approach to solve this complex problem?

The newton approach ?

Possible but ... heavy and dirty calculus

$$\Sigma \overrightarrow{F} = m \overrightarrow{a}$$

$$\delta S = \delta \int_{t_0}^{t_1} \mathscr{L}(x, y, z, \dot{x}, \dot{y}, z, \dot{x}, \dot{y}, z, \dot{y}, \dot{y}$$









Optical/mechanical equivalence: a simple example











Discovery of electrons and the beginning of electron optics

Joseph John Thomson (1856- m. 1940)

« Cathode rays (1897) »

Discovery of electrons. Trajectories of these particles deflected by an electric or magnetic field.







• Louis de Broglie (1892-m. 1987) « Recherches sur la théorie des quanta (1905) »











Variational methods to study charged particles trajectories

Integral picture of classical mechanics : definition of **action** S $\delta S = \delta \int_{t_0}^{t_1} \mathscr{L}(x, y, z, \dot{x}, \dot{y}, \dot{z}, t) dt = 0$



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Lagrangian of a charged particle Q in an EM field (\overrightarrow{A}, U)

$$\mathscr{L} = m_r c^2 \left(1 - \sqrt{1 - (v^2/c^2)} \right) + Q \left(\overrightarrow{v} \cdot \overrightarrow{A} - U \right)$$

$$\Rightarrow \quad \text{Considering a static field}} \quad \mathscr{L} = const$$

$$\tilde{S} = S + E(t - t_0) = \int_{z_0}^{z} \tilde{\mathscr{L}} dz, \qquad \qquad L = \frac{\tilde{S}}{q_0} = \int_{z_0}^{z} \mu dz \implies \mu =$$

Least action principle in static field equivalent to Fermat's principe in conventional optic considering $\mu =$





The characteristic function of light and of charged particles : optical index INSA



$$\delta L = \delta \int_{z_0}^{z} \left(n(x, y, z) \sqrt{1 + x^2 + y^2} \right) dz = 0 \quad \Rightarrow \quad \delta L = \delta \int_{z_0}^{z} \frac{1}{q_0} \overrightarrow{p} \frac{d\overrightarrow{r}}{dz} dz = 0 \quad \Rightarrow \quad \mu = \frac{1}{q_0} \left(m\overrightarrow{v} \cdot \frac{d\overrightarrow{r}}{dz} - e\overrightarrow{A} \cdot \frac{d\overrightarrow{r}}{dz} \right) = \mu_e + \mu_$$









Introduction to charged particle optics

Field and action expansion Definition of the optical index for charged particles

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We have to generate a localized zone of potential: the lens for charged particles



Three electrodes : ground/voltage/ground





will act as a converging lens for the charged particles







Back to LAP: development of charged particle optics

• Walter Glaser (1906-m. 1960)

« Zur Bildfehlertheorie des Elektronenmikroskops » (1935).

First development of geometrical electron optics: based on the principle of least action

Zur Bildfehlertheorie des Elektronenmikroskops.	das gesuchte Seidelsche Eikonal. S_4 hat d
Von Walter Glaser in Prag.	$S_4 = -\frac{A}{4}R^2 - \frac{B}{4}\varrho^2 - C \varkappa^2 - \frac{D}{2}R\varrho + R$
Mit 2 Abbildungen. (Eingegangen am 16. August 1935.)	$+ F \rho \varkappa + G_{\circ \circ} R \sigma -$
Nach einer vereinfachten Herleitung der Bildfehler werden die drei Zerdrehungs- fehler ausführlich diskutiert und die Bezeichnungen: anisotropes Komma, anisotrope sphärische Aberration und anisotrope Verzeichnung dafür vor- geschlagen. Der Einfluß der Blendenstellung wird untersucht. Es wird das all- gemeine rotationssymmetrische optische Mittel kurz behandelt und ein not- wendiges und hinreichendes Kriterium für das identische Verschwinden der Zerdrehungsfehler angegeben.	Wenn wir die Differenz $n_1 s_1 g_1'^2 h_1'^2 - n_0 s_0 g_0'^2$ und analog mit anderen Differenzen verf Koeffizienten des Eikonals (56) folgende Fo $A = \frac{1}{2} \Delta n s g'^4 - \int_a^b [L g^4 + 2 M g^2 g'^2 + N g']$
	$B = \frac{1}{2} \Delta n s h'^4 - \int_a^b [L h^4 + 2 M h^2 h'^2 + N h]$
Von früher ²) her wissen wir, daß die Elektronenbewegung in einem elektromagnetischen Feld mit den Potentialen Φ und \mathfrak{A} äquivalent ist dem optischen Strahlengang in einem anisotropen Medium mit dem Brechungs-	$C = \frac{1}{2} \Delta n s g'^{2} h'^{2} - \int_{a}^{b} \left[L g^{2} h^{2} + 2 M g h g' h' \right]_{b}$
$\mu(\mathbf{r}, \mathbf{s}) = \sqrt{\Phi} + \eta(\mathfrak{A}\mathbf{s}), \eta = \sqrt{\frac{e}{2m}}.$ (1) Debei wird des Votentiel Φ von einem Punkte aus gezählt in dem die	$D = \frac{1}{2} \Delta n s g'^{2} h'^{2} - \int_{a}^{b} \left[L g^{2} h^{2} + M (g^{2} h'^{2} + g'^{2} h) \right]_{a}^{b}$
Elektronengeschwindigkeit Null ist. Die Elektronenstrahlen bestimmen sich somit aus dem Fermatschen Prinzip	$E = \frac{1}{2} \Delta n s g'^{3} h' - \int_{a}^{b} [L g^{3} h + M (g^{2} g' h' + b)]_{b}$
$\delta \int \mu \left(\mathfrak{r}, \mathfrak{s} \right) \mathrm{d} \sigma = 0. \tag{2}$	$F = \frac{1}{2} \Delta n s g' h'^{3} - \int_{a} [L g h^{3} + M (g h h'^{2} +$
The optical index	$G_{00} = \int_{a}^{b} \frac{1}{n} (P g^{2} - Q g'^{2}) dz, G_{01} = \int_{a}^{b} G_{11} = \int_{a}^{b} \frac{1}{n} (P h^{2} - Q h'^{2}) dz$
Particles Fermat's	
principie	





die Gestalt

 $E R \varkappa$

 $-2G_{01} \varkappa \sigma + G_{11} \varrho \sigma.$ (56) $h_0^{\prime 2} \operatorname{mit} \varDelta nsg^{\prime 2} h^{\prime 2}$ bezeichne fahren, erhalten wir für die ormeln:

 $h^{\prime 4}$] d z,

$$\left\{ \begin{array}{l} (57a) \\ (57b) \\ (57$$

Reminder of the characteristic function L for a charged particle in a static field



Decomposition of the characteristic function n into several parts: paraxial + aberrations : same work as <u>Schwarzschild</u> for conventional optics







(II) Taylor expansion of each Fourier component $\phi_{\nu}(r, \theta, z)$ and knowing that Laplace equations should be fulfilled for each Fourier component $\Delta \phi_{\nu} = 0$

$$\phi_0(r,z) = \Phi_0(z) + \Phi_0''(z) \times \frac{r^2}{4} + \Phi_0^{[4]}(z) \times \frac{r^4}{64} - \Phi_0^{[6]}(z) \times \frac{r^6}{2304} + \dots$$

Only axial potential $\Phi_0(z)$ and it's derivatives relative to z are needed !!

$$\oint \phi(r,\theta,z) = \sum_{\nu=0}^{\infty} \sum_{\lambda=0}^{\infty} \frac{(-1)^{\lambda} \times \nu! \times r^{2\lambda+\nu}}{4^{\lambda} \times \lambda! \times (\nu+\lambda)!} \times [\Phi_{\nu;r}^{[2\lambda]}(z) \times \cos(\nu \times \theta) + \Phi_{\nu;i}^{[2\lambda]}(z) \times \sin(\nu \times \theta)]$$
Fourier Taylor
$$\int \phi = \sum_{\nu=0}^{\infty} \sum_{\lambda=0}^{\infty} (-1)^{\lambda} \frac{\nu!}{\lambda!(\lambda+\nu)!} \left(\frac{w\overline{w}}{4}\right)^{\lambda} Re(\Phi_{\nu}^{[2\lambda]}(z)\overline{w}^{\nu}) \quad \Rightarrow \quad \text{A sum of poly}$$

• Notation
$$\Phi' = \frac{\partial \Phi}{\partial z}$$



 \Rightarrow Example of the rotationally symmetric component $\phi_0(r, z)$

olynomial functions.









Main applications of rotational symmetric field



Pierre Grivet (1911-m. 1992)

« Electrostatic Electron Microscope (1941) »



Electrostatic lenses in a TEM



Behind the development of the FIB (focused ion beam)



TOULOUSE

Development of the transmission electron microscope

Ernst August Friedrich Ruska (1906-m. 1988)

« Das Elektronenmikroskop (1932) »

Magnetostatic

(Mitteilung aus dem Hochspannungslaboratorium der Technischen Hochschule Berlin.)

Das Elektronenmikroskop.

Von M. Knoll und E. Ruska in Berlin.

Mit 11 Abbildungen. (Eingegangen am 16. Juni 1932.)

Die wichtigsten elektronenoptischen Abbildungssysteme und ihre Eignung für die vergrößerte Abbildung elektronenemittierender Objekte werden diskutiert. Die allgemeinen Bedingungen für fehlerfreie Bilder, Definition und Grenze des Auflösungsvermögens werden angegeben. Ein magnetisches Elektronenmikroskop mit kalter Kathode für schnelle Elektronen und die Ausführung magnetischer Linsen werden beschrieben und mehrere Mikrophotogramme wiedergegeben. Die Untersuchungsmethoden des Elektronenmikroskops und geeignete Abbildungssysteme für ein Ionenmikroskop werden besprochen.

Mikrophotogramme.

Fig. 8a zeigt ein über eine runde Blende gespanntes Molybdändrahtnetz, das durch ein mittels der Kondensorlinse konzentriertes Strahlbündel einer Metallentladungsröhre von hinten "beleuchtet" wurde. Zum Vergleich wurde in einem gewöhnlichen Projektionsmikroskop (Zeiss) dieselbe Netzblende in gleicher Vergrößerung aufgenommen (Fig. 8b). Man sieht, daß



Fig. 8a. Fig. 8b. Fig. 8. Vergleich zwischen elektronen- und lichtoptischer Abbildung. Molybdändrahtnetz, Drahtabstand 0,3 mm, 12 fach in einer Stufe auf vergoldetem Glasleuchtschirm vergrößert; Beschleunigungsspannung 70 kV. a) durch Elektronenmikroskop. b) durch normales Mikroskop.

Zur Erzeugung der Elektronenbilder auf dem am Boden des Metallrohres befindlichen Leuchtschirm dienen eisengekapselte Sammelspulen, die "Objektivspule" (mit einem möglichst kleinen Innendurchmesser), und die größere "Projektionsspule", welche das durch die Objektivspule in Höhe des Okularmikrometers erzeugte Zwischenbild weiter vergrößert. Eine Vergrößerung in zwei Stufen ergibt bei einer bestimmten geforderten



Gesamtvergrößerung bei gleicher kleinster Spulenbrennweite eine bedeutend kürzere Länge des Mikroskops; für geringe Vergrößerungen kommt man mit der Objektivspule allein aus. Die oberhalb der Objektivspule sichtbare "Kondensorspule" dient in Analogie zur Anordnung beim normalen Mikroskop zur Strahlsammlung der "Beleuchtungsquelle" auf das Objekt.

Als Leuchtschirm zur Sichtbarmachung der Elektronenbilder dient (wegen der großen Strukturfeinheit) bei schnelleren Elektronen (> 25 kV) eine Glasplatte, die durch Kathodenzerstäubung mit einer Metallschicht von etwa 100 m μ versehen ist³). Diese mit der Anode verbundene Schicht verhindert Fig. 5. Magnetisches Elektronenmikroskop die Aufladung des Schirms und erhöht durch Reflexion an dem Metallspiegel

die Lichtstärke der Fluoreszenzbilder. Der Glasschirm ist möglichst dünn (< 0,1 mm) zu wählen, damit er bei intensiver Bestrahlung unter der Er-



CNrs


Optical index expansion

 \rightarrow We have to start from the optical indices:







Keep polynomial functions of power $n \leq 2$ \rightarrow Paraxial optics with $L = L^0 + L^2$

Contribution of polynomial functions of power n > 2 — Aberrations $L^4 + \dots$







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Paraxial charged particle optics

Second order optical index Paraxial equations Electrostatic vs magnetostatic standard optics

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Paraxial optics: $n \leq 2$



Magnetostatic case

$$\mu_m^{(2)} = \frac{e}{q_0} Im \left(\frac{w\overline{w}}{4} \Psi_0''(z) + \frac{1}{2} \Psi_0'(z) \overline{w}w' - \Psi_2(z)\overline{w}^2 \right)$$

Electrostatic case

$$\mu_{e}^{(2)} = \frac{1}{2} \sqrt{\frac{\Phi_{0}^{*}(z)}{\Phi_{0}^{*}(z_{0})}} Re \left[w'\overline{w'} - \frac{w\overline{w}}{\Phi_{0}^{*}(z)} \left(\frac{\gamma_{0}\Phi_{0}''(z)}{4} + \frac{\Phi_{1}(z)\overline{\Phi}_{1}(z)}{8\Phi_{0}^{*}(z)} \right) + \frac{\overline{w}^{2}}{\Phi_{0}^{*}(z)} \left(\gamma_{0}\Phi_{2}(z) - \frac{w\overline{w}}{8\Phi_{0}^{*}(z)} \right) \right]$$







Paraxial straight axis optics : $n \leq 2$

2. Lagrange showed that this is equivalent

In paraxial, these equations become :

to resolve the set of Euler-Lagrange differential equations :
$$\frac{d}{dz}\frac{\partial\mu}{\partial\overline{w}'} - \frac{\partial\mu}{\partial\overline{w}} = 0$$
$$\frac{d}{dz}\frac{\partial(\mu^{(0)} + \mu^{(1)} + \mu^{(2)})}{\partial\overline{w}'} - \frac{\partial(\mu^{(0)} + \mu^{(1)} + \mu^{(2)})}{\partial\overline{w}} = 0$$

After inserting all the previous polynomial functions extracted from the field expansion we found « naturally » the paraxial equation of any charged particle optics system with straight optical axis :

$$\bullet w'' + \frac{\gamma_0}{2\Phi_0^*} (\Phi_0'' + iv_0 \Psi_0') w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{2\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\gamma_0}{2\Phi_0^*} \right) w' + \frac{\gamma_0}{2\Phi_0^*$$

We find again the contribution of Fourier components : Rotationally symmetric field $\nu = 0$

The **Wien condition** state that if an electrostatic dipolar field is applied in the system,







1. To determine the trajectories we simply have to resolve the least action principle applied to the characteristic function $\delta L = 0$



a magneto static dipolar field must be present to have a straight optic axis (w = 0). The relation between the two magnitudes should fulfill

$$\Phi_1 + iv_0\Psi_1 = 0$$









Dipolar field and Wien Filter as mass separator

• Dipolar field tilt the optical axis relatively : use to align the beam (known as deflectors) -100 V Φ 100 V • Application of Wien condition : the Wien filter $\Phi_1 + iv_0\Psi_1 = 0$ 0>0 $\vec{E} \otimes \vec{B}$ • An example of a Wien filter by students : fabrication and calculation Their realization Resolution of paraxial equation $\Phi_1, \Psi_1 = 0$ ----- Isotope 71Ga ----- Rayor marginal ----- Rayor principal colonne optique 200 400 Einzel lens Φ_0 Wien filter Φ_1, Ψ_1





Results in a Ga FIB (separation of isotopes)



Mass selection of the primary ions in FIB



Other application of EXB Wien filter in EM : monochromators (Thermofisher and Jeol)







Other applications of dipolar fields in curved axis optics : the sectors

<u>Beware</u> : Equations are slightly different as the field expansion cannot be performed using w = x + iy variables. You need to define new variables relative to the curved optic axis but the general idea remains the same.

See Rose's book to have the detail of the new field expansion, paraxial equations and aberrations



General overview



hemispherical

analyzer



- Focalisation and dispersion along one direction
- Nothing along the perpendicular direction

Application in EM : monochromator





Magnetostatic sector Application: mass analyser (for example SIMS)



- Focalisation and dispersion along one direction
- Nothing along the perpendicular direction

Application in EM : monochromator and Spectrometer (Gatan, Nion, CEOS, ...)





Let's start from the general paraxial equations ...

$$w'' + \frac{\gamma_0}{2\Phi_0^*} (\Phi_0' + iv_0 \Psi_0') w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_0}{2\gamma_0} \right) w' + \frac{\varphi_0}{2\gamma_0} \left(\Phi_0'' + iv_0 \Psi_0'' +$$

We assume $\Phi_1 = \Psi_1 = \Phi_2 = \Psi_2 = 0$. The paraxial equation is simplified with only $\nu = 0$ components contribution

$$w'' + \frac{\gamma_0}{2\Phi_0^*} (\Phi_0' + iv_0 \Psi_0') w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' \right) w = 0$$

We rewrite the complex coordinate system : $w(z) = u(z)e^{i\chi}$ defining the amplitude of the trajectory u(z) and the phase χ known as Larmor rotatio

Second-order differential equation (with varying factors)

$$u'' + \frac{\gamma_0 \Phi'_0}{2\Phi_0^*} u' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + \frac{e}{2m_e} \Psi_0'^2 \right) u = 0$$

There are 2 independent solutions :

Initial conditions : $u_{\alpha} \setminus u_{\alpha}(z_0) = 0, u'_{\alpha}(z_0) = 1$ Marginal ray/Axial ray $u_{\pi} u_{\pi}(z_0) = 1, u'_{\pi}(z_0) = 0$ Principal ray/Chief Ray/Field Ray

The solution for any ray is written as a simple linear combination of the two fundamental solutions : $u = c_1 u_{\alpha} + c_2 u_{\pi}$.

If $u_0 = u(z_0)$ and $u'_0 = u'(z_0)$ then we have $: u(z) = u'_0 u_\alpha(z) + u_0 u_\pi(z)$





$$\implies \chi = -\sqrt{\frac{e}{8m_e}} \int_{z_0}^z \frac{\Psi_0'}{\sqrt{\Phi_0^*}} dz$$









Paraxial properties of electrostatic lenses : the Einzel lens

Let's first consider a pure electrostatic system with rotational symmetry.

$$w'' + \frac{\gamma_0}{2\Phi_0^*} (\Phi_0' + iv_0 \Psi_0') w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' \right) w = 0 \implies$$
$$x'' + \frac{1}{2} \frac{\Phi_0'}{\Phi_0^*} x' + \frac{1}{4} \frac{\Phi_0''}{\Phi_0^*} x$$

3. Extract axial potential $\Phi_0(z)$ 4. Compute $\Phi'_{0}(z), \Phi''_{0}(z)$



1.Define geometry and voltages

2. Calculate potential distribution





23 Runge–Kutta Methods

The idea of generalizing the Euler method, by allowing for a number of evaluations of the derivative to take place in a step, is generally attributed to Runge (1895). Further contributions were made by Heun (1900) and Kutta (1901). The latter completely characterized the set of Runge–Kutta methods of order 4, and proposed the first methods of order 5. Special methods for second order differential equations were proposed by Nyström (1925), who also contributed to the development of methods for first order equations. It was not until the work of Huťa (1956, 1957) that sixth order methods were introduced.

Since the advent of digital computers, fresh interest has been focused on Runge–Kutta methods, and a large number of research workers have contributed to recent extensions to the theory, and to the development of particular methods. Although early studies were devoted entirely to explicit Runge-Kutta methods, interest has now moved to include implicit methods, which have become recognized as appropriate for the solution of stiff differential equations.



We have $\Psi_0 = 0$, and we can extract two equations as w(z) = x(z) + iy(z)





5. Resolve paraxial equation using R-K algorithm

230 Historical introduction

A number of different approaches have been used in the analysis of Runge-Kutta methods, but the one used in this section, and in the more detailed analysis of Chapter 3, is that developed by the present author (Butcher, 1963), following on from the work of Gill (1951) and Merson (1957).

6. Draw the 2 fundamental rays from which any ray can be obtained



Simulation of an electrostatic column







General overview of the FIB column





Paraxial properties of magnetostatic lenses : the electromagnetic lens

Paraxial equation for magnetic system with rotational symmetry $(\Psi_0 \neq 0, \Phi_0 = 0)$

$$w(z) = x(z) + iy(z) = u(z)e^{i\chi}$$

$$u'' + \frac{\gamma_0}{4\Phi_0^*} \left(\frac{e}{2m_e} {\Psi_0'}^2\right) u = 0$$

Simplified paraxial equation
$$u'' + k^2(z)u = 0$$

1.Define geometry and voltages 2.Calculate potential distribution 3.Extract axial field $\Psi'_0(z) = B(z)$



- 4. Resolve paraxial equation using R-K algorithm
- 5. Plot trajectories in (x, y, z) space.
- Due to Larmor rotation not easy to visualise





Larmor rotation

$$\chi = -\sqrt{\frac{e}{8m_e}} \int_{z_0}^{z} \frac{\Psi_0'(z)}{\sqrt{\Phi_0^*}} dz = -\frac{1}{2} \frac{Q}{\sqrt{2K_0m}} \int_{z_0}^{z} B(z)$$
Focal distance

$$\frac{1}{f} = \frac{Q^2}{8K_0m} \int_{z_0}^{z_i} B^2(z) dz > 0$$

$$\Rightarrow No \text{ diverging lens}$$



Simulation of a complete magnetostatic TEM column

Marginal ray of a double lens system in (u, z)











Paraxial properties of electrostatic lenses : overview of immersion system INSA





Energy change between object and image area

$$\mu_{e}^{(0)} = \sqrt{\frac{\Phi_{0}^{*}(z)}{\Phi_{0}^{*}(z_{0})}} \neq \frac{1}{f}$$

$$\frac{1}{f} \approx \frac{3}{16} \left(\frac{\Phi_{0}(z_{0})}{\Phi_{0}(z_{i})}\right)^{\left(\frac{1}{4}\right)} \int_{z_{0}}^{z_{i}} \frac{\Phi_{0}(z_{0})}{\Phi_{0}(z_{i})}$$

Energy not change between object and image area

$$\mu_e^{(0)} = \sqrt{\frac{\Phi_0^*(z)}{\Phi_0^*(z_0)}} = \frac{1}{f} \approx \frac{3}{16} \int_{z_0}^{z_i} \frac{\Phi_0'^2(z)}{\Phi_0(z)^2} dz$$

K = 1000 eV

















(<u>[</u>]]}

The Schottky field emission (SFE) electron source

General overview

Tip + suppressor



The SFE assembly









CNrs

Let's start from the general paraxial equations ...

$$w'' + \frac{\gamma_0}{2\Phi_0^*} (\Phi_0' + iv_0 \Psi_0') w' + \frac{\gamma_0}{4\Phi_0^*} \left(\Phi_0'' + iv_0 \Psi_0'' + \frac{\Phi_1 \overline{\Phi}_1}{2\gamma_0 \Phi_0^*} \right) w - \frac{\gamma_0}{\Phi_0^*} \left(\Phi_2 + iv_0 \Psi_2 - \frac{\Phi_1^2}{8\gamma_0 \Phi_0^*} \right) \overline{w} = \frac{\gamma_0}{2\Phi_0^*} (\Phi_1 + iv_0 \Psi_1)$$

$$w(z) = x(z) + iy(z)$$
We assume $\Phi_1 = \Psi_1 = \Phi_0 = \Psi_0 = 0$. The paraxial equation is simplified with only the contribution of the $\nu = 2$ component $x'' + k^2 x = 0$

$$y'' - k^2 y = 0$$
A. Electrostatic quadrupole
$$k = k_E = \sqrt{(e\Phi_2)/(Kr_0^2)}$$
B. Magnetostatic quadrupole
$$k = k_M = \sqrt{(2e\Psi_2)/(pr_0^2)}$$
Periodic solutions along x :

Periodic solutions along x:

$$x(z) = x_0 cos(kz) + \frac{a_0}{k} sin(kz)$$

$$a(z) = -x_0 ksin(kz) + a_0 cos(kz)$$
Diverging solutions along y:

$$y(z) = y_0 cosh(kz) + \frac{a_0}{k} sinh(kz)$$

$$b(z) = y_0 cosh(kz) + \frac{a_0}{k} sinh(kz)$$

$$b(z) = y_0 ksinh(kz) + b_0 cosh(kz)$$













Correction of deviation from rotation symmetry : the stigmator

A. Electrostatic quadrupole



B. Magnetostatic quadrupole



Paraxial action of quadrupoles are used to compensate small paraxial focusing error along perpendicular directions observed in rotational system (electrostatic or magnetic)



Often called « Axial astigmatism » (not an aberration coming from $L^{(4)} + \ldots$ terms of the eikonal)





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Stigmatic imaging with quadrupoles multiplets

• Quadrupoles doublet : anamorphic focusing





• Quadrupoles quadruplet (Russian quadruplet) : non-anamorphic focusing (like round lens)







Electron Energy Loss Spectrometer : EELS



Post-column spectrometer









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Electron Energy Loss Spectrometer : EELS













Paraxial properties : to remember



What about the aberrations ?



Magnetostatic • Round and quadrupole can focus • Action depends on beam impulsion/charge (mass dependent) • Can be used to separate mass, not adapted to focus heavy ions • Magnetic material properties important (hysteresis, saturation,...)







Effect of fourth order terms L^4 of the expansion : Scherzer's theorem

After Glaser's work on aberrations expansion arrive ...

• Otto Scherzer (1909-m. 1982)

« Uber einige Fehler von Elektronenlinsen» (1936).

Über einige Fehler von Elektronenlinsen.

Von 0. Scherzer in Darmstadt.

Mit 3 Abbildungen. (Eingegangen am 4. Juni 1936.)

Unmöglichkeit des Achromaten. Die Bildfehler dritter Ordnung. Unvermeidbarkeit der sphärischen Aberration.

$$\begin{split} C_s &= \frac{1}{16} \int_{z_o}^{z_i} \Big\{ b^4 h^4 + 2 \big(h b' + h' b \big)^2 h^2 + 2 b^2 h^2 h'^2 \} dz \\ C_c &= \frac{1}{4} \int_{z_o}^{z^i} b^2 h^2 dz \end{split}$$

4. Unvermeidbarkeit der sphärischen Aberration.

He shows that if we have a system define by static rotationally fields :

$$\Psi_0 \neq 0, \Phi_0 \neq 0$$

This is known as *Scherzer's theorem*





Aberration terms of the eikonal expansion are unavoidable

$$L = L^0 + L^2 + L^4 + \dots > 0$$





Cancel fourth order terms L^4 of the expansion : Scherzer's propositions

• Otto Scherzer (1909-m. 1982)

« Sphärische und chromatische Korrektur von Elektronen-Linsen » (1947).

Scherzer shows that octopole field $\nu = 4$ can be used to invert the sign of spherical aberration

Sphärische und chromatische Korrektur von **Elektronen-Linsen.** Von O. Scherzer, z. Zt. USA (Aus den Süddeutschen Laboratorien in Mosbach.) (Mit 7 Textabbildungen.) Die Brauchbarkeit des Elektronenmikroskops bei hohen Vergrößerungen wird durch den Öffnungsfehler und die chromatische Aberration beeinträchtigt. Beide Fehler sind unvermeidlich, solange die abbildenden Felder rotations-symmetrisch, ladungsfrei und zeitlich konstant sind. Die vorliegende Untersuchung soll zeigen, daß die Aufhebung irgendeiner dieser drei Einschränkungen genügt, um den Weg zur sphärischen und chromatischen Korrektur und damit zu einer erheblichen Steigerung des Auflösungsvermögens freizugeben.

Solange nicht klar zu sehen ist, welche Art Linsen das beste Mikroskop ergibt, müssen alle sich bietenden Wege verfolgt werden. Es scheint daher angebracht, etwas ausführlicher auf die verschiedenen Arten korrigierter Linsen einzugehen.











Hexapole Ψ_3, Φ_3



Octopole Ψ_4, Φ_4





Cancel fourth order terms L^4 of the expansion : Rose's proposition



Harald Rose (1935-)

« Outline of a spherically corrected semiaplanatic medium-voltage transmission electron microscope» (1990).

Design of the first TEM and STEM spherical aberration corrected optics (semiaplanatic)

Harald Rose Geometrical **Charged-Particle Optics** 2nd Edition

D Springe

Springer Series in Optical Sciences 142





Students of Pr. Rose have the created the CEOS GmbH company























Currently: instrument optically limited by L^6 and not yet the diffraction limit









5 Aberrations in Charged particles optics

High order optical index Wavefront aberrations Scherzer theorem Correction of spherical aberration

([[]])



Aberrations (n > 2): n = 4 Seidel or primary geometric aberrations

Below, the indices obtained have been expressed for the round contributions Ψ_0, Φ_0 and quadripolar Ψ_2 only ...

4th order magneto static index

$$\begin{split} \mu_{\sigma}^{(4)} &= -\frac{e}{q_{0}} Re^{\left\{ W_{0}^{2} W_{0}^{2} \left[\frac{i}{12} W_{2}^{2} u_{u}^{4} + \frac{i}{6} W_{2} u_{u}^{2} \left(u_{u}^{2} + i x^{2} u_{u} \right) \right] e^{-2k}} \right\}} \\ & \mu_{\sigma}^{(4)} &= -\frac{e}{q_{0}} Re^{\left\{ W_{0}^{2} W_{0}^{2} \left[\frac{i}{12} W_{2}^{2} u_{u}^{4} + \frac{i}{6} W_{2} u_{u}^{2} \left(u_{u}^{2} + i x^{2} u_{u} \right) \right] e^{-2k}} \right\}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{12} W_{2}^{2} u_{u}^{4} + \frac{i}{6} W_{2} u_{u}^{2} \left(u_{u}^{4} + i x^{2} u_{u} \right) \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{12} W_{2}^{2} u_{u}^{4} + \frac{i}{6} W_{2} u_{u}^{2} \left(u_{u}^{4} + i x^{2} u_{u} \right) \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{12} W_{2}^{2} u_{u}^{4} + \frac{i}{6} W_{2} u_{u}^{2} \left(u_{u}^{4} + i x^{2} u_{u} \right) \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{12} W_{2}^{2} u_{u}^{4} + \frac{i}{6} W_{2} u_{u}^{2} \left(u_{u}^{4} + i x^{2} u_{u} \right) \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{12} W_{2}^{2} u_{u}^{4} + \frac{i}{2} W_{2} u_{u}^{2} u_{u}^{4} + i x^{2} u_{u}^{4} \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{2} u_{u}^{2} u_{u}^{4} + \frac{i}{2} W_{2} u_{u}^{2} u_{u}^{4} + i x^{2} u_{u}^{4} \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{2} u_{u}^{2} u_{u}^{4} + \frac{i}{2} W_{2} u_{u}^{2} u_{u}^{4} + i x^{2} u_{u}^{4} \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{2} u_{u}^{2} u_{u}^{4} + \frac{i}{2} W_{2} u_{u}^{2} u_{u}^{4} + i x^{2} u_{u}^{4} \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{2} u_{u}^{2} u_{u}^{4} + \frac{i}{2} W_{2} u_{u}^{2} u_{u}^{4} + i x^{2} u_{u}^{4} \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{0}^{2} u_{u}^{4} + \frac{i}{2} W_{2} u_{u}^{2} u_{u}^{4} + i x^{2} u_{u}^{4} \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{0}^{2} u_{u}^{4} + \frac{i}{2} W_{2} u_{u}^{2} u_{u}^{4} (u_{u}^{4} + i x^{2} u_{u}^{4}) \right] e^{-2k}} \\ & + u_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{0}^{2} u_{u}^{4} + i x^{2} u_{u}^{2} \right] + \frac{i}{2} W_{2}^{2} u_{u}^{4} u_{u}^{2} (u_{u}^{4} + i x^{2} u_{u}^{4}) \right] e^{-2k}} \\ & + w_{0}^{2} W_{0}^{2} \left[\frac{i}{4} W_{0}^{2} u_{u}^{4} u_{u}^{2} u_{u}^{2} u_{u}^{2} + i x^{2} u_{u}^{2} u_{u}^{4} u_{u}^{2} u$$

• After Scherzer, we can show that Ψ_3, Φ_3 and Ψ_4, Φ_4 can be used to cancel out the aperture aberration caused by Ψ_0, Φ_0 (see Pr. Rose's book for details)

4th order electrostatic index

- Rotationnaly symetric field Ψ_0, Φ_0 induce :
- Aperture aberration (spherical)
- Fields aberrations :
 - ► Coma,
 - ▶ Petzval curvature,
 - Field astigmatism
 - Distorsion
- Quadrupolar component Ψ_2 induces :
- Aperture aberrations (star and rosette)
- Fields aberrations (many comas terms, ...)

FIG. 7. Third-order comas. (a) Conjugate coma; (b) elliptical coma; (c) conjugate elliptical coma. The fourth row down shows the aberration figures in the Gaussian image plane, and the other rows, the same figures as they appear in other current planes. (From Burfoot, 1956.)

Wavefront aberrations: the most common aperture terms

Object point (no field) in the optical axis (such as a SEM, TEM, STEM or FIB source). We then assume $\overline{w}_0 = 0, w_0 = 0$

$$W = \frac{\tilde{S}}{q_0} = \int_{z_0}^{z} \mu dz \implies Re \left[A_0 \overline{w}_0' + \frac{1}{2} C_{df} |w_0'|^2 + \frac{1}{2} A_1 \overline{w}_0'^2 + \overline{B}_2 |w_0'|^2 \overline{w}_0' + \frac{1}{3} A_2 \overline{w}_0'^3 + \frac{1}{4} C_s |w_0'|^4 + \overline{S}_3 |w_0'|^2 \overline{w}_0'^2 \right]$$

Equations intégrales des coefficients $A_0 = \frac{ie}{a_0} \int_{z_1}^{z} (u_{\alpha} \Psi_1 e)^{i\chi} dz$ • Beam tilt $C_{df} = \int_{z_0}^{z} \left| \sqrt{\frac{\Phi_0^*}{\Phi_0^*(z_0)}} \left(u_{\alpha}^{'2} + \chi^{'2} u_{\alpha}^2 - \frac{\gamma_0}{4\Phi_0^*} \Phi_0^{''} u_{\alpha}^2 \right) + \frac{e\chi'}{q_0} \Psi_0' u_{\alpha}^2 \right| dz$ • Defocus $A_1 = \frac{2ie}{a_0} \int_{-\infty}^{z} \Psi_2 u_d^2 e^{-2i\chi} dz \quad \bullet \text{ Axial astigmatism (ordre 1)}$ $\overline{B}_2 = -\frac{ie}{4q_0} \int_{z_0}^z dz \left[\underbrace{\frac{1}{2} \Psi_1'' u_\alpha^3}_{z_0} + \Psi_1 \left(u_\alpha^2 u_\alpha' + i\chi' u_\alpha^3 \right) \right] e^{-i\chi}$ Axial Coma $A_2 = \frac{3ie}{a_0} \int_{-3i\chi}^{z} \Psi_3 u_d^2 e^{-3i\chi} dz \quad \bullet \text{Axial astigmatism(ordre 2)}$ $C_{s} = \frac{1}{2} \int_{z_{0}}^{z} dz \left[\sqrt{\frac{\Phi_{0}^{*}}{\Phi_{0}^{*}(z_{0})}} \left(-\left(u_{\alpha}^{'2} + \chi^{'2}u_{\alpha}^{2}\right)^{2} - \frac{\gamma_{0}}{2\Phi_{0}^{*}} \Phi_{0}^{''}u_{\alpha}^{2} \left(u_{\alpha}^{'2} + \chi^{'2}u_{\alpha}^{2}\right) \right] \right) + Spherical aberration$ $+\frac{1}{16}\left(\gamma_{0}\Phi_{0}^{''''}+\frac{\Phi_{0}^{''2}}{\Phi_{0}^{*}}\right)u_{\alpha}^{4}-\frac{1}{2q_{0}}\Psi_{0}^{'''}\chi'u_{\alpha}^{4}$ $\overline{S}_3 = -\frac{ie}{q_0} \int_{-\pi}^{\pi} dz \left[\frac{\Psi_2''}{6} u_{\alpha}^4 + \frac{\Psi_2'}{3} (u_{\alpha}' + i\chi' u_{\alpha}) u_{\alpha}^3 \right] e^{-2i\chi} \quad \cdot \text{ Star}$

We obtain a sum of polynomials functions of different orders depending on the variables of the entrance pupil (\overline{w}'_0, w'_0). Each function is weighted by an aberration coefficient :

Polynomial sum gives the final wavefront

Overview of the general method to study a CPO element

How does it work in practice? evaluation of the terms in the field

- - To do this, we need to solve the Laplace equation (differential equation) starting from the boundary conditions:

The first step is to calculate and map the potential (electrostatic or magnetostatic or both) in the volume of your optical element in 3D.

Dirichlet (fixed potential on the surface of the electrodes) or Neumann (field $\vec{E} \cdot \vec{n}$ fixed on the surface of the electrodes, \vec{n} being the normal to the surface)

There are 3 main strategies for solving these differential equations:

How does it work in practice? evaluation of the terms in the field

 $\Phi_{\nu} = -$

Once the potential ϕ,ψ has been determined in 3D, we can extract the various multipolar components Φ_{ν},Ψ_{ν} using ϕ,ψ derivatives :

- We can then solve the paraxial equation :
- $w'' + \frac{\gamma_0}{2\Phi_0^*} (\Phi_0' + iv_0 \Psi_0') w' + \frac{\gamma_0}{4\Phi_0^*}$
- To achieve this, numerical integration methods of the Runge-Kutta 4 type are generally used.
- We then plot the two paraxial solutions (marginal, principal)
 - 2.0 ······ Rayon principal ---- rayon marginal 1.5 1.0 0.5 y (mm) -0.5-1.0 -1.5 z (mm)

Calculation of Φ_{ν}, Ψ_{ν} derivatives along the z axis and then integrating the integration to determine aberrations (integration using numerical methods such as Simps

$$\frac{2-\delta_{o\nu}}{\nu!} \left(\frac{\partial^{\nu}\phi}{\partial\bar{w}^{\nu}}\right)_{w=0} \in \mathbb{C}$$

$$\left(\Phi_0'' + iv_0\Psi_0'' + \frac{\Phi_1\overline{\Phi}_1}{2\gamma_0\Phi_0^*}\right)w - \frac{\gamma_0}{\Phi_0^*}\left(\Phi_2 + iv_0\Psi_2 - \frac{\Phi_1^2}{8\gamma_0\Phi_0^*}\right)\overline{w} = \frac{\gamma_0}{2\phi_0^*}(\Phi_1 + iv_0\Psi_1)$$

23 Runge–Kutta Methods

230 Historical introduction

The idea of generalizing the Euler method, by allowing for a number of evaluations of the derivative to take place in a step, is generally attributed to Runge (1895). Further contributions were made by Heun (1900) and Kutta (1901). The latter completely characterized the set of Runge–Kutta methods of order 4, and proposed the first methods of order 5. Special methods for second order differential equations were proposed by Nyström (1925), who also contributed to the development of methods for first order equations. It was not until the work of Huťa (1956, 1957) that sixth order methods were introduced.

Since the advent of digital computers, fresh interest has been focused on Runge–Kutta methods, and a large number of research workers have contributed to recent extensions to the theory, and to the development of particular methods. Although early studies were devoted entirely to explicit Runge–Kutta methods, interest has now moved to include implicit methods, which have become recognized as appropriate for the solution of stiff differential equations.

A number of different approaches have been used in the analysis of Runge-Kutta methods, but the one used in this section, and in the more detailed analysis of Chapter 3, is that developed by the present author (Butcher, 1963), following on from the work of Gill (1951) and Merson (1957).

egral equations
son's method).
$$\blacktriangleright C_s = \frac{1}{2} \int_{z_0}^{z} dz \left[\sqrt{\frac{\Phi_0^*}{\Phi_0^*(z_0)}} \left(-\left(u_{\alpha}^2 + \chi^2 u_{\alpha}^2\right)^2 - \frac{\gamma_0}{2\Phi_0^*} \Phi_0'' u_{\alpha}^2 \left(u_{\alpha}^2 + \chi^2 u_{\alpha}^2\right) + \frac{1}{16} \left(\gamma_0 \Phi_0''' - \frac{\Phi_0''^2}{\Phi_0^*} \right) u_{\alpha}^4 \right) - \frac{e}{2q_0} \left[\sqrt{\frac{\Phi_0^*}{\Phi_0^*(z_0)}} \left(-\left(u_{\alpha}^2 + \chi^2 u_{\alpha}^2\right)^2 - \frac{\gamma_0}{2\Phi_0^*} \Phi_0'' u_{\alpha}^2 \left(u_{\alpha}^2 + \chi^2 u_{\alpha}^2\right) + \frac{1}{16} \left(\gamma_0 \Phi_0''' - \frac{\Phi_0''^2}{\Phi_0^*} \right) u_{\alpha}^4 \right] - \frac{e}{2q_0} \right] dz$$

How does it work in practice? evaluation of the terms in the field

Calculation of the EM field and determination of the on-axis field (FEM for EOD) : 1.

Paraxial solutions: marginal + principal (Runge-Kutta) 2.

Electron Optical Design SPOC - Software for Particle Optics Computations

iso, aniso distortion:

iso, aniso chromatic:

axial chromatic:

3. **Paraxial properties + aberrations**

Computation	with	asympto	otic obje	ect		
V*	=	1.0000	0000E+00) V		
U	=	1.0000	0000E+00) eV		
image #	=	1 (as	symptotic	2)		
z obje c t	=	-5.000	00000	mm		
z image	=	60.	.0000	mm		
rotation	=	0.000	00000	rad		
		0.000	00000	deg		
dir. magnif.	=	-6.21	16739			
ang. magnif.	=	-0.160	08560			
V* object	=	1.0000	00000E+00	V (
V* image	=	1.0000	0000E+00	V (
1-M*Ma*sqrt(p(zi)/p(zo)) = -5.29420952E-12						
fproj	=	9.082	20777	mm		
zproj	=	3.539	90932	mm		
Aberration c	oeffi	cients	related	to obj	ect	
Aberration c axial spher	oeffi ical	cients aber.:	related 9.0529	to obj 9E+01	ect	mm
Aberration c axial spher iso,aniso c	oeffi ical oma l	cients aber.: .ength:	related 9.0529 8.9722	to obj)E+01 LE+00,	ect 0.0000E+00	mm
Aberration c axial spher iso,aniso c field curva	oeffi ical oma l ture:	cients aber.: ength:	related 9.0529 8.9722 1.1784	to obj E+01 E+00, E+00	ect 0.0000E+00	mm 1/mm
Aberration c axial spher iso,aniso c field curva iso,aniso a	oeffi ical oma l ture: stigm	cients aber.: .ength: natism:	related 9.0529 8.9722 1.1784 2.5496	to obj E+01 E+00, E+00 E-01,	ect 0.0000E+00 0.0000E+00	mm 1/mm 1/mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d	oeffi ical oma l ture: stigm istor	cients aber.: ength: natism: tion:	related 9.0529 8.9727 1.1784 2.5496 4.6112	to obj 9E+01 1E+00, 1E+00 5E-01, 2E-02,	ect 0.0000E+00 0.0000E+00 0.0000E+00	mm 1/mm 1/mm 1/mm^2
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom	oeffi ical oma l ture: stigm istor atic:	cients aber.: ength: natism: tion:	related 9.0529 8.9722 1.1784 2.5496 4.6112 1.2484	to obj E+01 E+00, E+00 5E-01, E-02, E+02	ect 0.0000E+00 0.0000E+00 0.0000E+00	mm 1/mm 1/mm 1/mm^2 mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c	oeffi ical oma l ture: stigm istor atic: hroma	cients aber.: ength: natism: tion:	related 9.0529 8.9722 1.1784 2.5496 4.6112 1.2484 6.6222	to obj E+01 E+00, E+00 5E-01, 2E-02, E+02, E+00,	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	mm 1/mm 1/mm 1/mm^2 mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c	oeffi ical oma l ture: stigm istor atic: hroma	cients aber.: ength: natism: tion:	related 9.0529 8.9723 1.1784 2.5496 4.6112 1.2484 6.6222	to obj E+01 E+00, E+00 5E-01, 2E-02, E+02 2E+00,	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	mm 1/mm 1/mm 1/mm^2 mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c Aberration c	oeffi ical oma l ture: stigm istor atic: hroma	cients aber.: ength: natism: tion: ntic: cients	related 9.0529 8.9723 1.1784 2.5496 4.6112 1.2484 6.6222	to obj E+01 E+00, E+00 5E-01, E-02, E+02 E+00, Cture	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	mm 1/mm 1/mm 1/mm ² mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c Aberration c Aperture pos	oeffi ical oma l ture: stigm istor atic: hroma oeffi ition	cients aber.: ength: natism: tion: tic: cients at z=	related 9.0529 8.9721 1.1784 2.5496 4.6112 1.2484 6.6222 for aper 0.00	to obj 2E+01 1E+00, 1E+00 5E-01, 2E-02, 1E+02 2E+00, cture 000000E	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	mm 1/mm 1/mm^2 mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c Aberration c Aperture pos ra = 1	oeffi ical oma l ture: stigm istor atic: hroma oeffi ition .1462	cients aber.: ength: natism: tion: tic: cients at z= E+01,	related 9.0529 8.9723 1.1784 2.5496 4.6112 1.2484 6.6222 for aper 0.00 rb =	to obj 2E+01 2E+00, 4E+00 5E-01, 2E-02, 4E+02 2E+00, 5ture 000000E 1.0872	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 +00 mm E+00	mm 1/mm 1/mm^2 mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c Aberration c Aperture pos ra = 1	oeffi ical oma l ture: stigm istor atic: hroma oeffi ition .1462	cients aber.: ength: natism: tion: tic: cients at z= E+01,	related 9.0529 8.9722 1.1784 2.5496 4.6112 1.2484 6.6222 for aper 0.00 rb =	to obj 2E+01 2E+00, 4E+00 5E-01, 2E-02, 4E+02 2E+00, cture 000000E 1.0872	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 +00 mm E+00	mm 1/mm 1/mm^2 mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c Aberration c Aperture pos ra = 1 axial spher	oeffi ical oma l ture: stigm istor atic: hroma oeffi ition .1462	cients aber.: ength: natism: tion: tic: cients at z= E+01, aber.:	related 9.0529 8.9723 1.1784 2.5496 4.6112 1.2484 6.6222 for aper 0.00 rb = 9.0529	<pre>to obj E+01 E+00, E+00 5E-01, 2E-02, E+02 2E+00, Cture 000000E 1.08722 0E+01</pre>	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 +00 mm E+00	mm 1/mm 1/mm^2 mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c Aberration c Aperture pos ra = 1 axial spher iso,aniso c	oeffi ical oma 1 ture: stigm istor atic: hroma oeffi ition .1462 ical oma 1	cients aber.: ength: natism: tion: tic: cients at z= E+01, aber.: ength:	related 9.0529 8.9723 1.1784 2.5496 4.6112 1.2484 6.6222 for aper 0.00 rb = 9.0529 -8.2012	<pre>to obj E+01 E+00, E+00, E-01, E-02, E+02 E+02 E+00, Cture 000000E 1.0872 E+01 E+01 E+00,</pre>	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 +00 mm E+00 0.0000E+00	mm 1/mm 1/mm ² mm
Aberration c axial spher iso,aniso c field curva iso,aniso a iso,aniso d axial chrom iso,aniso c Aberration c Aperture pos ra = 1 axial spher iso,aniso c field curva	oeffi ical oma 1 ture: stigm istor atic: hroma oeffi ition .1462 ical oma 1 ture:	cients aber.: ength: natism: tion: tic: cients at z= 2E+01, aber.: ength:	related 9.0529 8.9723 1.1784 2.5496 4.6112 1.2484 6.6222 for aper 0.00 rb = 9.0529 -8.2012 1.1053	<pre>to obj e+01 E+00, E+00, E+00, E-02, E+02 E+02 E+00, Cture 000000E 1.0872 E+01 E+00, BE+00</pre>	ect 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 +00 mm E+00 0.0000E+00	mm 1/mm 1/mm^2 mm mm

1.2484E+02

-1.4315E-02, 0.0000E+00 1/mm²

-5.2188E+00, 0.0000E+00

Introduction to main aberration corrector solutions

Quadrupole-octopole solution Hexapole solution

([]]}

How can we correct aberrations ? The Scherzer move

• Otto Scherzer (1909-m. 1982)

« Sphärische und chromatische Korrektur von Elektronen-Linsen » (1947).

Sphärische und chromatische Korrektur von **Elektronen-Linsen.**

Von O. Scherzer, z. Zt. USA.

(Aus den Süddeutschen Laboratorien in Mosbach.) (Mit 7 Textabbildungen.)

Die Brauchbarkeit des Elektronenmikroskops bei hohen Vergrößerungen wird durch den Öffnungsfehler und die chromatische Aberration beeinträchtigt. Beide Fehler sind unvermeidlich, solange die abbildenden Felder rotations-symmetrisch, ladungsfrei und zeitlich konstant sind. Die vorliegende Untersuchung soll zeigen, daß die Aufhebung irgendeiner dieser drei Einschränkungen genügt, um den Weg zur sphärischen und chromatischen Korrektur und damit zu einer erheblichen Steigerung des Auflösungsvermögens freizugeben.

Solange nicht klar zu sehen ist, welche Art Linsen das beste Mikroskop ergibt, müssen alle sich bietenden Wege verfolgt werden. Es scheint daher angebracht, etwas ausführlicher auf die verschiedenen Arten korrigierter Linsen einzugehen.

Wir erhalten so für die durch das Korrekturfeld hervorgerufenen Verschiebungen in der Bildebene in Analogie zu (2,4):

$$\begin{aligned} \mathbf{x}_{b\,\mathbf{k}} &= \frac{-\mathrm{V}}{\sqrt{\Phi_{\mathbf{a}}}} \int_{\mathbf{z}_{\mathbf{a}}}^{\mathbf{z}_{b}} \frac{\varepsilon_{\mathbf{x}} \, \mathbf{x}_{a}}{\sqrt{\Phi}} \, \mathrm{d} \, \mathbf{z} = \frac{2 \, \mathrm{V}}{\sqrt{\Phi_{\mathbf{a}}}} \int_{\mathbf{z}_{\mathbf{a}}}^{\mathbf{z}_{b}} \frac{\Phi_{\mathbf{a}}}{\sqrt{\Phi}} (3 \, a \, \beta^{2} \, \mathbf{x}_{a}^{2} \, \mathbf{y}_{a}^{2} - a^{3} \, \mathbf{x}_{a}^{4}) \, \mathrm{d} \, \mathbf{z}; \\ \mathbf{y}_{b\,\mathbf{k}} &= \frac{-\mathrm{V}}{\sqrt{\Phi_{\mathbf{a}}}} \int_{\mathbf{z}_{\mathbf{a}}}^{\mathbf{z}_{b}} \frac{\mathrm{sy} \, \mathbf{y}_{a}}{\sqrt{\Phi}} \, \mathrm{d} \, \mathbf{z} = \frac{2 \, \mathrm{V}}{\sqrt{\Phi_{\mathbf{a}}}} \int_{\mathbf{z}_{\mathbf{a}}}^{\mathbf{z}_{b}} \frac{\Phi_{\mathbf{a}}}{\sqrt{\Phi}} (3 \, a^{2} \, \beta \, \mathbf{x}_{a}^{2} \, \mathbf{y}_{a}^{2} - \beta^{3} \, \mathbf{y}_{a}^{4}) \, \mathrm{d} \, \mathbf{z}; \\ \text{Die Korrekturforderung} \, \mathbf{x}_{b\mathbf{u}} + \mathbf{x}_{b\mathbf{k}} = 0; \, \mathbf{y}_{b\mathbf{u}} + \mathbf{y}_{b\mathbf{k}} = 0 \text{ ist nun ver} \end{aligned}$$

mäßig einfach zu erfüllen. Ein negatives Φ_4 an einer Stelle, wo $x_a y_a \neq 0$ ist, bringt nach (3,2) und (3,4) den Koeffizienten von $\alpha \beta^2$ und, wegen

Combinaison of Φ_2, Ψ_2 (for paraxial) and Φ_4, Ψ_4 for spherical aberration correction

The quadrupoles/octopoles solution

Quadrupole-Octopole association

NION dedicated STEM

• Vernon D. Beck (Albert Crewe's group in Chicago) « A hexapole spherical aberration corrector» (1978).

The semiaplanatic double hexapoles solution

• Harald Rose (1935-m. ?)

« Outline of a spherically corrected semiaplanatic medium-voltage transmission electron microscope» (1990).

Hexapole correction

Optik 85, No. 1 (1990) 19-24 © Wissenschaftliche Verlagsgesellschaft mbH, Stuttgart

Outline of a spherically corrected semiaplanatic medium-voltage transmission electron microscope

H. Rose

Insitut für Angewandte Physik Technische Hochschule Darmstadt, FRG

Outline of a spherically corrected semiaplanatic medium-volt-Outline of a spherically corrected semiaplanatic medium-volt-age transmission electron microscope. A spherically corrected semiaplanatic objective lens for a subangstrom medium-voltage transmission electron microscope (TEM) is outlined. The aplanatic corrector consists of two telescopic round-lens doublets and two sextupoles centered about the nodal points of the second doublet. If the corrector is incorporated into a 300 kV TEM equipped with a field emission gun a resolution limit of 0.6 Å and 10⁴ equally-well-resolved image points per diameter can be obtained. For achieving this performance the magnetic field of the objective lens must be stabilized with a relative accuracy of 1 ppm, while the fields of the corrector elements require at most a stability of 10 ppm

racy has prevented a successful improvement of the resolution by these correctors.

The amount of expenditure necessary for correction reduces considerably if the chromatic aberration can be kept below 1 Å. In this case only the spherical aberration must be compensated. Contrary to the chromatic aberration the spherical aberration can be corrected by sextupole elements which do not affect the paraxial path of rays. This possibility is of great advantage because the fields of the sextupole elements need only to be stabilized with a relative accuracy of about 10^{-4} in the case of atomic resolution

Corrector off

Short hexapoles

Long hexapoles

({[]]}}

The semiaplanatic double hexapoles solution













Introduction to symplectic relations in CPO

Canonical equations of Hamilton Optics as a canonical transformation Symplectic geometry and relations between coefficients due to symplecticity







Geometrical optics as a canonical transformation

ON A GENERAL METHOD OF EXPRESSING THE PATHS OF LIGHT, AND OF THE PLANETS, BY THE COEFFICIENTS OF A CHARACTERISTIC FUNCTION

By

William Rowan Hamilton

Dublin University Review and Quarterly Magazine, 1 (1833), pp. 795–826.)



THEORY OF SYSTEMS OF RAYS

By

William Rowan Hamilton

(Transactions of the Royal Irish Academy, vol. 15 (1828), pp. 69–174.)

Notation

The Poisson's bracket

 $\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t}$

 $\delta S = \delta \int_{t_0}^{t_1} \mathscr{L}(\vec{r}, \dot{\vec{r}}, t) dt = 0$ LAP : Canonical momentum : $\vec{p} = \frac{\partial \mathscr{L}}{\vec{r}}$ Hamiltonian :

> After integration by parts we find the two canonical Hamilton's equation of motion (they simply replace the Euler-Lagrange equations which are not canonical)

Canonial base In object space (r_i, p_i)

 ${f, g}_{(r_i, p_i)}$



$$\{f, g\}_{(r_i, p_i)} = \{$$

The Poisson's bracket rules of canonical basis

$$\{r_i, p_j\} = \delta_{ij}$$
$$\{r_i, r_j\} = 0$$
$$\{p_i, p_j\} = 0$$





([[]])

Geometrical optics as a canonical transformation : $t \rightarrow z$

Using z as time, it's better to define the canonical transformation which transform $(x, p_x) \rightarrow (X(x, p_x, z), P_X(x, p_x, z))$ in two separate 2D planes

We define the matrix known as phase-space vector :

$$\mathbf{X}(z) = (x(z), p_x(z), y(z), p_y(z), E, t(z))$$





Phase-Space mapping of a beam profile : Emittance diagram



Emittance evolution in an optical system : example





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Canonical geometrical optics : the symplectic relations

The symplectic transformation is define by the following metric relation for each phase-space vector :

		Aka <u>S</u>	ymplect	<u>ic relatio</u>	<u>ns</u>		
	I is the J	acobian n	natrix of	the phase	e space va	ariables	
-	two phas	se-space	« time » 2	z_0 and z_1	(object ar	nd imag	Э)
		dr /dn	Notation) dr (dn	dr /dK	0)	
	dr Idr						
	$\partial x_1 / \partial x_0$	$\partial x_1 / \partial p_{x0}$	$\partial x_1 / \partial y_0$	$\frac{\partial v_1}{\partial y_0}$	$\partial x_1 / \partial K_0$		
	$\partial x_1 / \partial x_0$ $\partial p_{x1} / \partial x_0$	$\partial p_{x1} / \partial p_{x0}$	$\partial p_{x1}/\partial y_0$	$\partial p_{x1}/\partial p_{y0}$	$\partial p_{x1} / \partial K_0$	0	
_	$\frac{\partial x_1}{\partial x_0}$ $\frac{\partial p_{x1}}{\partial x_0}$ $\frac{\partial y_1}{\partial x_0}$	$\partial x_1 / \partial p_{x0}$ $\partial p_{x1} / \partial p_{x0}$ $\partial y_1 / \partial p_{x0}$	$\frac{\partial p_{x1}}{\partial y_0}$ $\frac{\partial p_{x1}}{\partial y_0}$	$\partial p_{x1} / \partial p_{y0}$ $\partial y_1 / \partial p_{y0}$	$\partial p_{x1} / \partial K_0$ $\partial y_1 / \partial K_0$	0	
II	$\frac{\partial x_1}{\partial x_0}$ $\frac{\partial p_{x1}}{\partial x_0}$ $\frac{\partial y_1}{\partial x_0}$ $\frac{\partial p_{y1}}{\partial x_0}$	$\frac{\partial p_{x1}}{\partial p_{x0}}$ $\frac{\partial p_{x1}}{\partial p_{x0}}$ $\frac{\partial p_{y1}}{\partial p_{x0}}$	$\frac{\partial p_{x1}}{\partial y_0}$ $\frac{\partial p_{y1}}{\partial y_0}$ $\frac{\partial p_{y1}}{\partial y_0}$	$\frac{\partial p_{x1}}{\partial p_{y0}}$ $\frac{\partial p_{x1}}{\partial p_{y0}}$ $\frac{\partial p_{y1}}{\partial p_{y0}}$	$\frac{\partial p_{x1}}{\partial K_0}$ $\frac{\partial p_{y1}}{\partial K_0}$ $\frac{\partial p_{y1}}{\partial K_0}$	0 0 0	
=	$\frac{\partial x_1}{\partial x_0}$ $\frac{\partial p_{x1}}{\partial x_0}$ $\frac{\partial y_1}{\partial x_0}$ $\frac{\partial p_{y1}}{\partial x_0}$ 0	$\frac{\partial p_{x1}}{\partial p_{x0}}$ $\frac{\partial p_{x1}}{\partial p_{x0}}$ $\frac{\partial p_{y1}}{\partial p_{x0}}$ $\frac{\partial p_{y1}}{\partial p_{x0}}$	$\frac{\partial p_{x1}}{\partial y_0}$ $\frac{\partial p_{y1}}{\partial y_0}$ $\frac{\partial p_{y1}}{\partial y_0}$ 0	$\frac{\partial p_{x1}}{\partial p_{y0}}$ $\frac{\partial p_{x1}}{\partial p_{y0}}$ $\frac{\partial p_{y1}}{\partial p_{y0}}$ $\frac{\partial p_{y1}}{\partial p_{y0}}$	$\frac{\partial p_{x1}}{\partial K_0}$ $\frac{\partial p_{y1}}{\partial K_0}$ $\frac{\partial p_{y1}}{\partial K_0}$ $\frac{1}{2}$	0 0 0 0	



Geometric operation which conserve Poisson's bracket are **symplectic transformation**







Symplectic relations taking care of non linear coefficients

Nuclear Instruments and Methods in Physics Research A238 (1985) 127-140 North-Holland, Amsterdam

RELATIONS BETWEEN ELEMENTS OF TRANSFER MATRICES DUE TO THE CONDITION OF SYMPLECTICITY

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Received 30 January 1985

More than 100 relations up to third order coefficients ...

SYMMETRY-BASED DESIGN OF FRAGMENT SEPARATOR ... Phys. Rev. ST Accel. Beams 10, 064002 (2007 $-2(a|x\delta)(x|xa) + 2(a|xa)(x|x\delta) + (a|xa\delta)(x|x) - (a|x)(x|xa\delta) - (a|xx\delta)(x|a) + (a|a)(x|xx\delta) = 0$ $-2(a|x\delta)(x|aa) + 2(a|aa)(x|x\delta) + (a|aa\delta)(x|x) - (a|x)(x|aa\delta) - (a|xa\delta)(x|a) + (a|a)(x|xa\delta) = 0$ $2(a|a\delta)(x|x\delta) - 2(a|x\delta)(x|a\delta) + (a|a\delta\delta)(x|x) - (a|x)(x|\delta\delta a) - (a|x\delta\delta)(x|a) + (a|a)(x|x\delta\delta) = 0$ 2(b|ay)(y|xy) - 2(b|xy)(y|ay) + (a|ayy)(x|x) - (a|x)(x|ayy) - (a|xyy)(x|a) + (a|a)(x|xyy) = 0-2(b|xy)(y|ab) + 2(b|ab)(y|xy) + (a|ayb)(x|x) - (a|x)(x|ayb) - (a|xyb)(x|a) + (a|a)(x|xyb) = 02(b|ay)(y|xb) - 2(b|xb)(y|ay) - (a|x)(x|ayb) + (a|ayb)(x|x) - (a|xyb)(x|a) + (a|a)(x|xyb) = 0-2(b|xb)(y|ab) + 2(b|ab)(y|xb) - (a|x)(x|abb) + (a|abb)(x|x) - (a|xbb)(x|a) + (a|a)(x|xbb) = 0-2(b|xy)(y|ay) + 2(b|ay)(y|xy) - (b|y)(y|xay) + (b|xay)(y|y) - (a|xyy)(x|a) + (a|a)(x|xyy) = 0-2(b|xy)(y|ab) + 2(b|ab)(y|xy) - (b|y)(y|xab) + (b|xab)(y|y) - (a|xyb)(x|a) + (a|a)(x|xyb) = 0-(b|y)(y|aay) + (b|aay)(y|y) - (a|ayy)(x|a) + (a|a)(x|ayy) = 0-2(b|ay)(y|ab) + 2(b|ab)(y|ay) - (b|y)(y|aab) + (b|aab)(y|y) - (a|ayb)(x|a) + (a|a)(x|ayb) = 0 $-2(b|y\delta)(y|ay) + 2(b|ay)(y|y\delta) + (b|ay\delta)(y|y) - (b|y)(y|ay\delta) - (a|yy\delta)(x|a) + (a|a)(x|yy\delta) = 0$ $-2(b|y\delta)(y|ab) + 2(b|ab)(y|y\delta) + (b|ab\delta)(y|y) - (b|y)(y|ab\delta) - (a|yb\delta)(x|a) + (a|a)(x|yb\delta) = 0$ -2(a|yy)(x|xa) + 2(a|xa)(x|yy) + (b|xay)(y|y) - (b|y)(y|xay) - (a|xyy)(x|a) + (a|a)(x|xyy) = 0-2(a|yy)(x|aa) + 2(a|aa)(x|yy) + (b|aay)(y|y) - (b|y)(y|aay) - (a|ayy)(x|a) + (a|a)(x|ayy) = 0 $2(a|a\delta)(x|yy) - 2(a|yy)(x|a\delta) + (b|ay\delta)(y|y) - (b|y)(y|ay\delta) - (a|yy\delta)(x|a) + (a|a)(x|yy\delta) = 0$ -2(a|yb)(x|xa) + 2(a|xa)(x|yb) - (b|y)(y|xab) + (b|xab)(y|y) - (a|xyb)(x|a) + (a|a)(x|xyb) = 0-2(a|yb)(x|xa) + 2(a|xa)(x|yb) - (b|y)(y|xab) + (b|xab)(y|y) - (a|xyb)(x|a) + (a|a)(x|xyb) = 0-2(a|yb)(x|aa) + 2(a|aa)(x|yb) - (b|y)(y|aab) + (b|aab)(y|y) - (a|ayb)(x|a) + (a|a)(x|ayb) = 0 $2(a|a\delta)(x|yb) - 2(a|yb)(x|a\delta) - (b|y)(y|ab\delta) + (b|ab\delta)(y|y) - (a|yb\delta)(x|a) + (a|a)(x|yb\delta) = 0$ 2(a|yy)(x|xx) - 2(a|xx)(x|yy) + (a|xyy)(x|x) - (a|x)(x|xyy) + (b|y)(y|xxy) - (b|xxy)(y|y) = 0-2(a|xx)(x|yb) + 2(a|yb)(x|xx) + (a|xyb)(x|x) - (a|x)(x|xyb) + (b|y)(y|xxb) - (b|xxb)(y|y) = 02(a|yy)(x|xa) - 2(a|xa)(x|yy) - (a|x)(x|ayy) + (a|ayy)(x|x) + (b|y)(y|xay) - (b|xay)(y|y) = 0-2(a|xa)(x|by) + 2(a|by)(x|xa) - (a|x)(x|ayb) + (a|ayb)(x|x) + (b|y)(y|xab) - (b|xab)(y|y) = 0 $2(a|yy)(x|x\delta) - 2(a|x\delta)(x|yy) + (a|yy\delta)(x|x) - (a|x)(x|yy\delta) + (b|y)(y|xy\delta) - (b|xy\delta)(y|y) = 0$ $-2(a|x\delta)(x|yb) + 2(a|yb)(x|x\delta) + (a|yb\delta)(x|x) - (a|x)(x|yb\delta) + (b|y)(y|xb\delta) - (b|xb\delta)(y|y) = 0$ 064002-11

Notation $(x \mid a) = \partial x(z) / \partial a_0$ $(b | xx) = (1/2!)(\partial^2 b(z)/\partial x_0^2)$





 $(T \mid aa) = -\frac{p_1^{ref}}{K_0^{ref}}(x \mid a\delta)M_a$







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Some books to conclude







Conventional optics



Charged particles optics



Bibliotherapy







CINC

Thank you

