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电多极透镜的束流光学

胡 酉 雄　　　西 门 纪 业
（南京大学物理系，210008）　（北京大学无线电系，100871）

摘　　要

本文推导了电多极透镜的象差矩阵 ΔM，并证明 $|\Delta M + I| = 1$，在此基础上考虑象差时，只要对束流相椭球进行适当修正，束的传输仍可按相椭球规则进行，从而建立了电多极透镜的束流光学。

一、引　　言

在许多电子和离子光学系统中聚焦带电粒子和修正象差是一个主要的课题。为了这个目的常常采用电多极透镜。人们利用它的四极电场对电子(离子)进行一级聚焦，六极电场修正二级象差，八极电场修正三级象差。例如利用它在加速器系统中做传输元件，在电子束器件和电子显微镜中做聚焦透镜和消象散器以及球差矫正器等。本文作者之一西门纪业曾考虑了具有象差的各种电子光学元件以及它们的组合场的束流光学[1-4]，本文将研究同时存在二级和三级象差的上述三个电场叠加形成的电多极透镜的束流光学。 文中首先推导出二级和三级象差系数的积分公式，并证明二级和三级象差同时存在的情况下带电粒子所占据的相空间体积不变。随后将二级和三级象差引起的微扰合理地引入束流特性矩阵中，使得在考虑象差的影响时仍保持了束流特性矩阵的椭球传输特点。从而建立起考虑象差的电多极透镜的束流光学。

二、电多极透镜的电场

图 1 给出了一个直角坐标系。 假设在 z_0 与 z 之间存在一个电多极透镜，由它所产生的空间电位 φ 应该满足拉氏方程：

$$\Delta\varphi(x,y,z) = 0. \tag{1}$$

如果把电位 $\varphi(x,y,z)$ 围绕 z 轴展成幂级数则可写作：

$$\varphi(x, y, z) = \sum_{m,n=0}^{\infty} a_{m,n} x^m y^n. \tag{2}$$

将(2)式代入(1)式，并考虑到 x 和 y 的平权性，就可以得

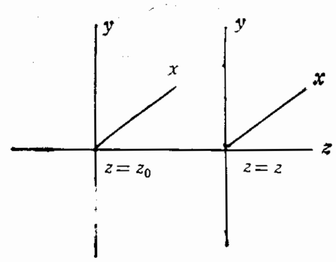

图 1　直角坐标系

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到电多极透镜的电位表达式为[5]

$$\varphi = V + \frac{1}{4}Q(x^2 - y^2) + E\left(\frac{1}{3}x^3 - xy^2\right) + P(x^4 + y^4) - 6Px^2y^2, \tag{3}$$

式中 V 是带电粒子进入电多极透镜的加速电压，Q 是正则四极场场强参数，E 是六极场场强参数，P 是正则的八极场场强参数．它们都是 z 的函数，如果将它们与 z 的关系用场的中心部分场强和增加电多极透镜的有效长度来代替，那末 Q、E、P 就与 z 无关，从而电多极透镜也就变成一个不考虑边缘场的硬边界透镜．

三、粒子运动方程

从[6]可知在电多极透镜中变分函数 F 为

$$F = \varphi^{\frac{1}{2}}(1 + x'^2 + y'^2)^{\frac{1}{2}}. \tag{4}$$

将(3)式代入，展开(4)式并保留四阶以前的各项，可以得到：

$$F = F_0 + F_2 + F_3 + F_4,$$

其中，

$$F_0 = V^{\frac{1}{2}};$$

$$F_2 = A(x^2 - y^2) + B(x'^2 + y'^2);$$

$$F_3 = C\left(\frac{1}{3}x^3 - xy^2\right);$$

$$F_4 = D(x^4 + y^4) - H(x^2 - y^2)^2 - 6Dx^2y^2 + \frac{B}{2}(x'^2 + y'^2)^2 + \frac{A}{2}(x^2 - y^2)(x'^2 + y'^2),$$

式中，

$$A = \frac{Q}{8V^{\frac{1}{2}}},\quad B = \frac{V^{\frac{1}{2}}}{2},\quad C = \frac{E}{2V^{\frac{1}{2}}},\quad D = \frac{P}{2V^{\frac{1}{2}}},\quad H = \frac{Q^2}{16V^{\frac{3}{2}}}.$$

由二级三级和四级变分函数就可得到直到三级的带电粒子的轨迹方程：

$$2Bx'' - 2Ax = C(x^2 - y^2) + 4Dx^3 - 4Hx(x^2 - y^2) - 12Dxy^2 + Ax(x'^2 + y'^2) + 2B(3x'^2x'' + x''y'^2 + 2y'y''x') + A(2xx'^2 + x^2x'' - 2yy'x' - x''y^2), \tag{5}$$

$$2By'' + 2Ax = -2Cxy + 4Dy^3 + 4Hy(x^2 - y^2) - 12Dx^2y - Ay(x'^2 + y'^2) + 2B(2x'x''y' + x'^2y'' + 3y'^2y'' + Ay''(x^2 - y^2) + Ay'(2xx' - 2yy'). \tag{6}$$

四、二级和三级象差

如果仅考虑一级近似，方程(5)和(6)变成

$$Bx'' - Ax = 0, \tag{7}$$

$$By'' + Ax = 0. \tag{8}$$

令：x_0, x'_0, y_0, y'_0 为带电粒子进入电多极透镜之前在 $z = z_0$ 处的起始位置和斜率，则方程

(7),(8)可以解出为:

$$\begin{cases} x = g_x x_0 + h_x x_0' \\ x' = g_x' x_0 + h_x' x_0' \end{cases}, \quad \begin{cases} y = g_y y_0 + h_y y_0' \\ y' = g_y' y_0 + h_y' y_0' \end{cases} \tag{9}$$

其中 g_x, h_x 和 g_y, h_y 为方程(7)和(8)的两对线性无关的特解。再根据文献[7]可以得到二级和三级象差的总和并表示为:

$$\begin{aligned} \Delta u &= h_u \int_{z_0}^{z} \left[\frac{\partial(F_3 + F_4)}{\partial u} g_u + \frac{\partial(F_3 + F_4)}{\partial u'} g_u' \right] dz \\ &\quad - g_u \int_{z_0}^{z} \left[\frac{\partial(F_3 + F_4)}{\partial u} h_u + \frac{\partial(F_3 + F_4)}{\partial u'} h_u' \right] dz, \\ \Delta u' &= h_u' \int_{z_0}^{z} \left[\frac{\partial(F_3 + F_4)}{\partial u} g_u + \frac{\partial(F_3 + F_4)}{\partial u'} g_u' \right] dz \\ &\quad - g_u' \int_{z_0}^{z} \left[\frac{\partial(F_3 + F_4)}{\partial u} h_u + \frac{\partial(F_3 + F_4)}{\partial u'} h_u' \right] dz, \end{aligned} \tag{10}$$

式中 $\Delta u = (\Delta x, \Delta y)$，$\Delta u' = (\Delta x', \Delta y')$。如果将方程组(10)中相同部分抽出来，并把一级近似解代入其中的 x, x', y, y'，然后按照 x_0, x_0', y_0, y_0' 的幂次分类排列后就可以得到:

$$\begin{aligned} \frac{\partial(F_3 + F_4)}{\partial u} g_u + \frac{\partial(F_3 + F_4)}{\partial u'} g_u' &= \sum_{\substack{\alpha,\beta,\gamma,\delta, \\ 2,4}} (\alpha,\beta,\gamma,\delta) x_0^{\alpha} x_0'^{\beta} y_0^{\gamma} y_0'^{\delta}, \\ \frac{\partial(F_3 + F_4)}{\partial u} h_u + \frac{\partial(F_3 + F_4)}{\partial u'} h_u' &= \sum_{\substack{\alpha,\beta,\gamma,\delta \\ 1,3}} (\alpha,\beta,\gamma,\delta) x_0^{\alpha} x_0'^{\beta} y_0^{\gamma} y_0'^{\delta}. \end{aligned} \tag{11}$$

(11)式左边对 x 求导对应右边求和符号 $\sum$ 的下标 1,2，对 y 求导对应求和符号$\sum$的下标 3,4，并且以下各象差系数括号外的下标也与它对应。式中 $2 \leqslant \alpha + \beta + \gamma + \delta \leqslant 3$，其中 $(\alpha,\beta,\gamma,\delta)$ 为二级或三级象差系数。现将求出的这些系数表示如下:

二级象差系数:

$(2000)_1$	$\int C g_x^2 h_x dz$	$(2000)_2$	$\int C g_x^3 dz$
$2(1100)_1$	$\int C g_x h_x^2 dz$	$2(1100)_2$	$\int C g_x^2 h_x dz$
$(0200)_1$	$\int C h_x^3 dz$	$(0200)_2$	$\int C h_x^2 g_x dz$
$(0020)_1$	$\int -C g_y^2 h_x dz$	$(0020)_2$	$\int -C g_x g_y^2 dz$
$2(0011)_1$	$\int -C g_y h_y h_x dz$	$2(0011)_2$	$\int -C g_x g_y h_y dz$
$(0002)_1$	$-\int C h_y^2 h_x dz$	$(0002)_2$	$-\int C g_x h_y^2 dz$
$(1010)_3$	$\int -2C g_x g_y h_y dz$	$(1010)_4$	$\int -2C g_x g_y^2 dz$
$(0110)_3$	$\int -2C h_x g_y h_y dz$	$(0110)_4$	$\int -2C g_y^2 h_x dz$
$(0101)_3$	$\int -2C h_x h_y^2 dz$	$(0101)_4$	$\int -2C h_x h_y g_y dz$

$(1001)_3 \quad \int -2Cg_x h_y^2 \mathrm{d}z \qquad (1001)_4 \quad \int -2Cg_x g_y h_y \mathrm{d}z$

三级象差系数:

为说明几何意义,按象差性质列出,其中的积分一律从 z_0 积到 z.

畸变:

$$(1020)=(0120)_2 \quad \int[4(H-3D)g_x g_y^2 h_x + Ag_x g_y'^2 h_x - 2Bg_x' g_y'^2 h_x' - Ag_y^2 g_x' h_x']\mathrm{d}z$$

$$\frac{1}{3}(2100)_2=(3000)_1 \quad \int[12(D-H)g_x^3 h_x + 3Ag_x^2 g_x' h_x' + 3g_x h_x g_x'^2 - 6Bg_x'^3 h_x']\mathrm{d}z$$

$$2(1011)_2 \quad \int[8(H-3D)g_x^2 g_y h_y + 2Ag_x^2 g_y' h_y' - 4Bg_x'^2 g_y' h_y' - 2Ag_x'^2 g_y h_y]\mathrm{d}z$$

$$(0030)_3=\frac{1}{3}(0021)_4 \quad \int[4(D+H)g_y^3 h_y - Ag_y g_y'^2 h_y - 2Bg_y'^3 h_y' - Ag_y^2 g_y' h_y']\mathrm{d}z$$

$$(2010)_3=(2001)_4 \quad \int[-4(H+3D)g_x^2 g_y h_y - Ag_x'^2 g_y h_y - 2Bg_x'^2 g_y' h_y' + Ag_x^2 g_y' h_y']\mathrm{d}z$$

$$(1110)_4 \quad \int[-8(H+3D)g_x g_y^2 h_x - 2Ag_x' g_y^2 h_x' + 2Ag_x g_y'^2 h_x - 4Bg_x' g_y'^2 h_x']\mathrm{d}z$$

象散:

$$(2100)_1=(1200)_2 \quad \int[12(D-H)g_x^2 h_x^2 + 4Ag_x g_x' h_x h_x' + Ag_x'^2 h_x^2 + Ag_x^2 h_x'^2 - 6Bg_x'^2 h_x'^2]\mathrm{d}z$$

$$2(1011)_1=2(0111)_2 \quad \int[8(H-3D)g_x g_y h_x h_y + 2Ag_x g_y' h_x h_y' - 2Ag_x' g_y h_x' h_y - 4Bg_x' g_y' h_x' h_y']\mathrm{d}z$$

$$(0021)_3=(0012)_4 \quad \int[12(D+H)g_y^2 h_y^2 - 4Ag_y g_y' h_y h_y' - 6Bg_y'^2 h_y'^2 - Ag_y'^2 h_y^2 - Ag_y^2 h_y'^2]\mathrm{d}z$$

$$2(1110)_3=2(1101)_4 \quad \int[-8(H+3D)g_x g_y h_x h_y - 2Ag_x' g_y h_x' h_y + 2Ag_x g_y' h_x h_y' - 4Bg_x' g_y' h_x' h_y']\mathrm{d}z$$

彗差:

$$\frac{1}{3}(1200)_1=(0300)_2 \quad \int[12(D-H)g_x h_x^3 + 3Ag_x h_x h_x'^2 + 3Ag_x' h_x' h_x^2 - 6Bg_x' h_x'^3]\mathrm{d}z$$

$$(1002)_1=(0102)_2 \quad \int[4(H-3D)g_x h_x h_y^2 + Ag_x h_x h_y'^2 - Ag_x' h_x' h_y^2 - 2Bg_x' h_x' h_y'^2]\mathrm{d}z$$

$$2(0111)_1 \quad \int[8(H-3D)g_y h_x^2 h_y + 2Ag_y' h_x^2 h_y' - 2Ag_y h_x'^2 h_y - 4Bg_y' h_x'^2 h_y']\mathrm{d}z$$

$$\frac{1}{3}(0012)_3=(0003)_4 \quad \int[12(D+H)g_y h_y^3 - 3Ag_y h_y h_y'^2 - 3Ag_y' h_y^2 h_y' - 6Bg_y' h_y'^3]\mathrm{d}z$$

$$2(1101)_3 \quad \int[-8(H+3D)g_x h_x h_y^2 - 2Ag_x' h_x' h_y^2 - 4Bg_x' h_x' h_y'^2 + 2Ag_x h_x h_y'^2]\mathrm{d}z$$

$$(0210)_3=(0201)_4 \quad \int[-4(H+3D)g_y h_x^2 h_y - Ag_y h_y h_x'^2 - 2Bg_y' h_x'^2 h_y' + Ag_y' h_x^2 h_y']\mathrm{d}z$$

球差:

$(0300)_1 \quad \int [4(D-H)h_x^4 + 2Ah_x^2h_x'^2 - 2Bh_x'^4]\mathrm{d}z$

$(0102)_1 \quad \int [4(H-3D)h_x^2h_y^2 + Ah_x^2h_y'^2 - 2Bh_y'^2h_x'^2 - Ah_x'^2h_y^2]\mathrm{d}z$

$(0003)_3 \quad \int [4(D+H)h_y^4 - 2Ah_y^2h_y'^2 - 2Bh_y'^4]\mathrm{d}z$

$(0201)_3 \quad \int [-4(H+3D)h_x^2h_y^2 - Ah_x'^2h_y^2 - 2Bh_x'^2h_y'^2 + Ah_x^2h_y'^2]\mathrm{d}z$

场曲：

$(0120)_1 \quad \int [4(H-3D)g_y^2h_x^2 + Ag_y'^2h_x^2 - 2Bg_y'^2h_x'^2 - Ag_y^2h_x'^2]\mathrm{d}z$

$(1002)_2 \quad \int [4(H-3D)g_x^2h_y^2 + Ag_x^2h_y'^2 - 2Bg_x'^2h_y'^2 - Ag_x'^2h_y^2]\mathrm{d}z$

$(2001)_3 \quad \int [4(H+3D)g_x^2h_y^2 - Ag_x'^2h_y^2 - 2Bg_x'^2h_y'^2 + Ag_x^2h_y'^2]\mathrm{d}z$

$(0210)_4 \quad \int [-4(H+3D)g_y^2h_x^2 - Ag_y^2h_x'^2 - 2Bg_y'^2h_x'^2 + Ag_y'^2h_x^2]\mathrm{d}z$

超畸变：

$(3000)_2 \quad \int [4(D-H)g_x^4 + 2g_x^2g_x'^2 - 2Bg_x'^4]\mathrm{d}z$

$(1020)_2 \quad \int [4(H-3D)g_x^2g_y^2 + Ag_x^2g_y'^2 - Ag_x'^2g_y^2 - 2Bg_x'^2g_y'^2]\mathrm{d}z$

$(0030)_4 \quad \int [4(D+H)g_y^4 - 2Ag_y^2g_y'^2 - 2Bg_y'^4]\mathrm{d}z$

$(2010)_4 \quad \int [-4(H+3D)g_x^2g_y^2 - Ag_x'^2g_y^2 + Ag_x^2g_y'^2 - 2Bg_x'^2g_y'^2]\mathrm{d}z.$

联合考虑方程(9)和(10)可以得到

$$\boldsymbol{x} = G(I + \Delta M)\boldsymbol{x}_0, \tag{12}$$

其中，

$$\boldsymbol{x} = \begin{vmatrix} x_1 + \Delta x \\ x_1' + \Delta x' \\ y_1 + \Delta y \\ y_1' + \Delta y' \end{vmatrix}, \quad \boldsymbol{x}_0 = \begin{pmatrix} x_0 \\ x_0' \\ y_0 \\ y_0' \end{pmatrix}, \quad G = \begin{vmatrix} g_x & h_x & 0 & 0 \\ g_x' & h_x' & 0 & 0 \\ 0 & 0 & g_x & h_y \\ 0 & 0 & g_y' & h_y' \end{vmatrix}, \quad I = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix},$$

$$\Delta M = \begin{vmatrix} \Delta M_{11} & \Delta M_{12} & \Delta M_{13} & \Delta M_{14} \\ \Delta M_{21} & \Delta M_{22} & \Delta M_{23} & \Delta M_{24} \\ \Delta M_{31} & \Delta M_{32} & \Delta M_{33} & \Delta M_{34} \\ \Delta M_{41} & \Delta M_{42} & \Delta M_{43} & \Delta M_{44} \end{vmatrix}.$$

I 是单位矩阵，ΔM 为象差矩阵，它的矩阵元为：

$$\Delta M_{11} = -[x_0(2000)_1 + x_0'(1100)_1 + x_0^2(3000)_1 + y_0^2(1020)_1 + x_0x_0'(2100)_1 + 2y_0y_0'(1011)_1 + x_0'^2(1200)_1 + y_0'^2(1002)_1];$$

$$\Delta M_{12} = -[x_0(1100)_1 + x_0'(0200)_1 + y_0^2(0120)_1 + 2x_0x_0'(1200)_1 + 2y_0y_0'(0111)_1$$

$$+ x_0'^2(0300)_1 + y_0'^2(0102)_1];$$

$$\Delta M_{13} = -[y_0(0020)_1 + y_0'(0011)_1];$$

$$\Delta M_{14} = -[y_0(0011)_1 + y_0'(0002)_1];$$

$$\Delta M_{21} = x_0(2000)_2 + x_0'(1100)_2 + x_0^2(3000)_2 + y_0^2(1020)_2 + 2x_0x_0'(2100)_2 + 2y_0y_0'(1011)_2 + y_0'^2(1002)_2;$$

$$\Delta M_{22} = x_0(1100)_2 + x_0'(0200)_2 + x_0^2(2100)_2 + y_0^2(0120)_2 + x_0x_0'(1200)_2 + 2y_0y_0'(0111)_2 + x_0'^2(0300)_2 + y_0'^2(0102)_2;$$

$$\Delta M_{23} = y_0(0020)_2 + y_0'(0011)_2;$$

$$\Delta M_{24} = y_0(0011)_2 + y_0'(0002)_2;$$

$$\Delta M_{31} = -[y_0(1010)_3 + y_0'(1001)_3];$$

$$\Delta M_{32} = -[y_0(0110)_3 + y_0'(0101)_3];$$

$$\Delta M_{33} = -[x_0(1010)_3 + x_0'(0110)_3 + x_0^2(2010)_3 + y_0^2(0030)_3 + 2x_0x_0'(1110)_3 + y_0'y_0(0021)_3 + x_0'^2(0210)_3 + y_0'^2(0012)_3];$$

$$\Delta M_{34} = -[x_0(1001)_3 + x_0'(0101)_3 + x_0^2(2001)_3 + 2x_0x_0'(1101)_3 + 2y_0y_0'(0012)_3 + y_0^{2\prime}(0003)_3 + x_0'^2(0201)_3];$$

$$\Delta M_{41} = y_0(1010)_4 + y_0'(1001)_4;$$

$$\Delta M_{42} = y_0(0110)_4 + y_0'(0101)_4;$$

$$\Delta M_{43} = x_0(1010)_4 + x_0'(0110)_4 + x_0^2(2011)_4 + y_0^2(0030)_4 + 2x_0x_0'(1110)_4 + 2y_0y_0'(0021)_4 + x_0'^2(0210)_4;$$

$$\Delta M_{44} = x_0(1001)_4 + x_0'(0101)_4 + x_0^2(2001)_4 + y_0^2(0021)_4 + 2x_0x_0'(1101)_4 + y_0y_0'(0012)_4 + x_0'^2(0201)_4 + y_0'^2(0003)_4.$$

从矩阵元中可以证明 $\Delta M_{11} + \Delta M_{22} = 0$，$\Delta M_{33} + \Delta M_{44} = 0$，也就是 $|\Delta M + I| = 1$，它意味着在考虑象差情况下刘维定理仍然成立。

五、电多极透镜的束流光学

文献[7、8]的微扰方法也可以用于电多极透镜，如果认为表征带电粒子束的相椭球在通过电多极透镜之后仍然保持椭球形，那末下式应该成立：

$$X^{T}\sigma^{-1}X = X_0^{T}(G + G\Delta M)^{T}\sigma^{-1}(G + G\Delta M)x_0 = x_0^{T}\sigma_0^{T}X_0, \tag{13}$$

式中 σ_0 为进入电多极透镜的带电粒子四维传输特征相椭球，σ 为从电多极透镜出来的特征相椭球，T为矩阵转置符号。

从公式(13)可知

$$\sigma_0^{-1} = (G + G\Delta M)^{T}\sigma^{-1}(G + G\Delta M),$$

$$\sigma = (G + G\Delta M)\sigma_0(G + G\Delta M)^{T}. \tag{14}$$

在忽略掉高阶项之后可以得到

$$\sigma = G\sigma_0G^{T} + G(\Delta M\sigma_0 + \sigma_0\Delta M^{T})G^{T}.$$

进一步设

$$\Delta\sigma_0 = \Delta M\sigma_0 + \sigma_0\Delta M^{T}, \tag{15}$$

则：

$$\sigma = G(\sigma_0 + \Delta\sigma_0)G^{T}. \tag{16}$$

从(15)式可以知道引起 $\Delta\sigma_0$ 的原因是象差矩阵 ΔM. 如果已知 σ_0 在 x 和 y 方向上彼此独立,即

$$\sigma_0 = \begin{vmatrix} \sigma_{011} & \sigma_{021} & 0 & 0 \\ \sigma_{021} & \sigma_{022} & 0 & 0 \\ 0 & 0 & \sigma_{033} & \sigma_{034} \\ 0 & 0 & \sigma_{043} & \sigma_{044} \end{vmatrix}.$$

那末由方程(15)可知

$$\Delta\sigma_{011} = 2(\Delta M_{11}\sigma_{011} + \Delta M_{12}\sigma_{012});$$

$$\Delta\sigma_{012} = \Delta\sigma_{021} = \Delta M_{21}\sigma_{011} + \Delta M_{12}\sigma_{022};$$

$$\Delta\sigma_{022} = 2(\Delta M_{21}\sigma_{012} + \Delta M_{22} + \sigma_{022});$$

$$\Delta\sigma_{033} = 2(\Delta M_{33}\sigma_{033} + \Delta M_{34}\sigma_{034});$$

$$\Delta\sigma_{034} = \Delta\sigma_{043} = (\Delta M_{43}\sigma_{033} + \Delta M_{34}\sigma_{044});$$

$$\Delta\sigma_{044} = 2(\Delta M_{43}\sigma_{034} + \Delta M_{44}\sigma_{044}).$$

到此为止本文已经建立起考虑象差的电多极透镜的束流光学.

参　考　文　献

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The Beam Optics of Electric Multipole Lens

Hu Naixiong

(Department of Physics, Nanjing University, 210008)

Ximen Jiye

(Department of Radio, Peking University, 100871)

Abstract

In this paper, the beam optics of an electric multipole lens containing aberrations is established, the aberration matrix is derived, and its determinant is shown to be unit. When the beam travels through an electric multipole lens and the aberrations exist, the electron beam theory for ellipsoid in phase space is still valid.