# Numerical simulation for space charge dominated beam transport*

Lü Jian-Qin(吕建钦)†

*State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing* 100871, *China*

(Received 26 November 2008; revised manuscript received 6 January 2009)

To simulate the intense bunched beam transport, a computer program LEADS-3D has been developed. The particle trajectories are analysed with the Lie algebraic method. The third order approximation of the trajectory solutions is made with space charge forces off, and the second order approximation is made with space charge forces on. The particle distribution in the 3D ellipsoid is uniform or Gaussian. Most of the conventional beam optical elements are incorporated in the code. The optimization procedures are provided to fit the beam lines to satisfy the given optical conditions.

**Keywords:** computer code, beam dynamics, intense bunched beam, nonlinear

**PACC:** 2921

## 1. General description of the code

LEADS-3D has evolved from an earlier code LEADS,[1] which was developed during the construction of the 4.5 MeV electrostatic accelerator at Peking University.[2] The original code, LEADS, may be used to calculate the beam optical systems consisting of drift space, electrostatic and magnetic quadrupoles, bending magnet, two-tube gap lens, three-tube Einzel lens, three-aperture Einzel lens and dc accelerating tube. The particle trajectories in these elements are calculated in the linear approximation. The old code can also be used to calculate quarter wave resonator (QWR) and split loop resonator (SLR) rf structures. The optimization procedures are provided to fit the beam lines to satisfy the given optical conditions. The old code offers graphical plotting of the phase space diagrams and beam envelopes.

Since then, more optical elements have been incorporated in the code, such as solenoid, sextupole, $\boldsymbol{E} \times \boldsymbol{B}$ cross field separator, cylindrical electrostatic analyser, and spherical electrostatic analyser. The third order terms of particle trajectories with space charge off and second order terms with space charge on have been added in the code for all of the optical elements. The new version of the code is named LEADS-3D.

## 2. Analysis of nonlinear particle trajectories with space charge off

### 2.1. Hamiltonian

#### 2.1.1. In Cartesian coordinate system

The Lie algebraic method[3] is used to generate a high-order symplectic map of the dynamical variables about the design trajectory (in practice up to the third order has been done). In the Cartesian system, when the particle beam moves in the $z$-direction, the Hamiltonian with time $t$ as the independent variable is

$$H_t = [m_0^2c^4 + c^2(p_x - qA_x)^2 + c^2(p_y - qA_y)^2 + c^2(p_z - qA_z)^2]^{1/2} + q\psi, \quad (1)$$

where $m_0$ is the rest mass of the particle; $q$ the charge; $c$ the light velocity in vacuum; $p_x$, $p_y$ and $p_z$ are the canonical particle momenta in the transverse and the longitudinal directions respectively; $A_x$, $A_y$ and $A_z$ the components of the applied magnetic vector potential; $\psi$ is the applied electrostatic potential. The electrostatic potentials and magnetic vector potentials for different optical elements are listed below.

**1) Electrostatic quadrupole focusing in $x$-plane**

$$\psi = \left(x^2 - y^2\right) V/r_0^2,$$

*Project supported by the National Natural Science Foundation of China (Grant No. 10975011), and the Specialized Research Fund for the Doctoral Program of Higher Education of China (Grant No. 20070001001).

†Corresponding author. E-mail: jqlu@pku.edu.cn

© 2010 Chinese Physical Society and IOP Publishing Ltd

where $V$ is the applied electric potential to the electrodes, $r_0$ is the inner radius, and

$$A_x = A_y = A_z = 0.$$

**2) Magnetic quadrupole focusing in $x$-plane**

$$\psi = 0,$$

and

$$A_x = A_y = 0, \quad A_z = \frac{G}{2}(y^2 - x^2),$$

where $G$ is the magnetic field gradient.

**3) Cylindrically symmetric electrostatic fields**[4]

$$\psi = \phi(z) - \frac{1}{4}\phi''(z)r^2 + \frac{1}{64}\phi^{(3)}(z)r^4 - \ldots,$$

where $\phi\ (z)$ is the electric potential distribution along the $z$-axis, and

$$A_x = A_y = A_z = 0.$$

**4) $\boldsymbol{E} \times \boldsymbol{B}$ cross field separator**

$$\psi = -v_0 x B,$$

where $v_0$ is the velocity of the reference particle, $B$ is the magnetic field, and

$$A_x = 0, \quad A_y = 0, \quad A_z = -xB.$$

**5) Sextupole**

$$\psi = 0,$$

and

$$A_x = 0, A_y = 0, \quad \text{and} \quad A_z = \frac{B_0}{a_0^2}(xy^2 - x^3/3),$$

where $a_0$ is inner radius, $B_0$ is the magnetic field.

**6) Solenoid**[5]

$$\psi = 0,$$

and

$$\begin{aligned} A_x &= -\frac{1}{2}By + \frac{1}{16}B''(x^2 + y^2)y, \\ A_y &= \frac{1}{2}Bx - \frac{1}{16}B''(x^2 + x^2)x, \\ A_z &= 0, \end{aligned}$$

where $B$ is the magnetic field distribution along the $z$ axis.

Now, introduce a new canonical variable $p_t$:

$$p_t = -H_t(x, y, z, p_x, p_y, p_z)$$

and work out $p_z$ from $p_t$, then one will obtain

$$\begin{aligned} K = -p_z = -[(p_t + q\psi)^2/c^2 - m_0^2c^2 - (p_x - qA_x)^2 \\ - (p_y - qA_y)^2]^{1/2} - qA_z. \end{aligned} \tag{2}$$

The function $K$ is a new Hamiltonian with $(x, p_x, y, p_y, t, p_t)$ as the canonical variables and $z$ as the independent variable.

Let

$$\begin{aligned} &x = r - r_0, \quad p_x = p_x, \quad y = y, \quad p_y = p_y, \\ &\tau = t - z/v_0, \quad p_\tau = p_t - p_t^0, \end{aligned}$$

where $p_t^0$ is the value of $p_t$ for the reference particle. In the new phase space $\boldsymbol{\zeta} = (x, p_x, y, p_y, \tau, p_\tau)$, the Hamiltonian is

$$\begin{aligned} H = -[&-(p_x - qA_x)^2 - (p_y - qA_y)^2 \\ &+ (p_t + p_t^0 + q\psi)^2/c^2 - m_0^2c^2]^{1/2} \\ &- qA_z - \frac{p_t + p_t^0}{v_0}. \end{aligned} \tag{3}$$

### 2.1.2. In curvilinear coordinate system

In the optical elements with curvilinear reference orbits (see Fig. 1), such as magnetic dipole, cylindrical electrostatic analyser and spherical electrostatic analyser, we use the curvilinear coordinate system ($x$, $y$, $\eta$), where $x$ is the particle displacement from the reference orbit in the radial direction, $y$ is the particle vertical position relative to the reference orbit, $\eta$ is the pass length of the designed orbit, $r_0$ is the radius of the designed orbit. The Hamiltonian of the particle motion is

$$\begin{aligned} H_t = c[&(p_r - qA_r)^2 + (p_y - qA_y)^2 \\ &+ (p_\phi/r - qA_\phi)^2 + m_0^2c^2]^{1/2} + q\psi, \end{aligned} \tag{4}$$

where $p_r$, $p_y$ and $p_\phi$ are the momentum components in the $r$, $y$ and $\eta$ directions respectively.

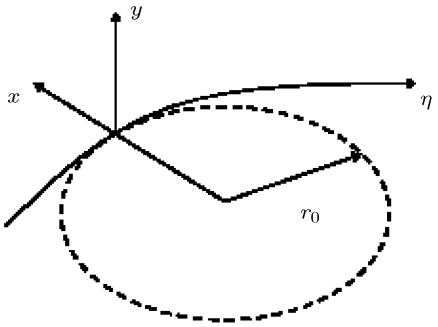



**Fig. 1.** The curvilinear.

The applied scalar potential and the vector potential for these elements are presented as follows.

**1) Magnetic dipole**

$$\psi = 0$$

and

$$A_x = A_y = 0, \quad A_\tau = -\frac{1}{2} r B_0.$$

**2) Cylindrical electrostatic potential**

$$\psi = \frac{m_0 \gamma_0 v_0^2}{q} \ln (x/r_0 + 1)$$

and

$$A_x = A_y = 0, \quad A_\tau = 0,$$

where $v_0$ and $r_0$ are the velocity and the orbit radius of the reference particle respectively, and $\gamma_0 = 1/\sqrt{1 - v_0^2/c^2}$.

**3) Spherical electrostatic potential**[6]

$$\psi = \frac{m_0 \gamma_0 v_0^2}{q} \left(1 - \frac{r_0}{r}\right)$$

and

$$A_x = A_y = 0, \quad A_\tau = 0.$$

Let

$$p_t = -H_t$$

and solve for $p_\phi$ from $p_t$, then one will have

$$K = -p_\phi = -r[(p_t + q\psi)^2/c^2 - (p_r - qA_r)^2 - (p_y - qA_y)^2 - m_0^2 c^2]^{1/2} - qrA_\phi.$$

The Hamiltonian $K$ is defined in the phase space ($r$, $p_r$, $y$, $p_y$, $t$, $p_t$) with curvilinear pass length $\tau$ as an independent variable. Now, introduce a new set of canonical variables:

$$\begin{aligned} &x = r - r_0, \quad y = y, \\ &\tau = t - \phi/\omega, \\ &p_x = p_r, \quad p_y = p_y, \\ &p_\tau = (p_t - p_t^0), \end{aligned}$$

where $\phi$ is the bending angle, $\omega$ the angle velocity of the reference particle, $p_0$ the momentum of the reference particle, $p_t^0$ the value of $p_t$ for the reference particle. In this case, the Hamiltonian is

$$H = -r_0 \left(1 + \frac{x}{r_0}\right) [(p_\tau + p_\tau^0 + q\psi)^2/c^2 - (p_x - qA_x)^2 - (p_y - qA_y)^2 - m_0^2 c^2]^{1/2} - qrA_\phi - (p_\tau - p_\tau^0)/\omega. \quad (5)$$

The canonical phase space for the function $H$ is $\varsigma = (x, p_x, y, p_y, \tau, p_\tau)$. In the both cases of Cartesian coordinate system and curvilinear coordinate system, the Hamiltonian in Eqs. (3) and (5) can all be expanded into Taylor series about the reference orbit as follows:

$$H = H_0 + H_1 + H_2 + H_3 + H_3 + \ldots. \quad (6)$$

## 2.2. Particle nonlinear trajectories

According to the principle of classical mechanics,[7] when the particle moves from the initial position $s_\mathrm{i}$ to the new position $s_\mathrm{f}$ along the reference orbit $s$ ($s$ can be straight reference obit $z$ or curvilinear reference obit $\eta$), its canonical coordinate $\varsigma = (x, p_x, y, p_y, \tau, p_\tau)$ will change from $\varsigma_\mathrm{i}$ to $\varsigma_\mathrm{f}$. This is a canonical transformation and can be expressed as follows:

$$\varsigma_\mathrm{f} = M\varsigma_\mathrm{i}, \quad (7)$$

where

$$M = \exp[: f :]$$

and

$$f = -\int_{q_\mathrm{i}}^{q_\mathrm{f}} H(\varsigma_\mathrm{i}, q)\mathrm{d}q.$$

$\mathfrak{M}$ is defined as Lie transformation associated with $H$. In general, a Lie transformation $\mathfrak{M}$ associated with an arbitrary function $f$ can be expressed as an exponential series

$$M = \sum_{n=0}^{\infty} : f :^n /n!.$$

Using the Dragt–Finn factorization theorem,[8] we have

$$\mathfrak{M} = \cdots \mathfrak{M} \cdot \mathfrak{M}_3 \cdot \mathfrak{M}_2, \quad (8)$$

where

$$\begin{aligned} &\mathfrak{M}_2 = \exp(: f_2 :), \quad \mathfrak{M}_3 = \exp(: f_3 :), \\ &\mathfrak{M}_4 = \exp(: f_4 :) \ldots \end{aligned} \quad (9)$$

and

$$\begin{aligned} f_2 &= -\int_{q_\mathrm{i}}^{q_\mathrm{f}} H_2 \mathrm{d}q, \\ f_3 &= -\int_{q_\mathrm{i}}^{q_\mathrm{f}} h_3^{\mathrm{int}}(\varsigma_\mathrm{i}, q)\mathrm{d}q, \\ f_4 &= -\int_{q_\mathrm{i}}^{q_\mathrm{f}} h_4^{\mathrm{int}}(\varsigma_\mathrm{i}, q)\mathrm{d}q \\ &\quad + \frac{1}{2}\int_{q_\mathrm{i}}^{q_\mathrm{f}} \mathrm{d}q_1 \int_{q_0}^{q_1} \mathrm{d}q_2 [-h_3^{\mathrm{int}}(\varsigma_\mathrm{i}, q_2), -h_3^{\mathrm{int}}(\varsigma_\mathrm{i}, q_1)], \\ &\quad \ldots \end{aligned} \quad (10)$$

and here

$$h_n^{\mathrm{int}}(\varsigma) = M_2 H_n. \quad (11)$$

In Eq. (8), $\mathfrak{M}_2$, $\mathfrak{M}_3$ and $\mathfrak{M}_4$ are the first order, second order and third order Lie maps.

Let $\varsigma_{\rm i}$ denote the initial particle coordinate in the phase space, $\varsigma_{\rm f}^j (j = 1, 2, 3, \ldots)$ represent the first, second and third orders of the final particle coordinate in the phase space, then the solutions of the equations of particle motion will be expressed as follows:

$$\begin{aligned} &\varsigma_{\rm f}^1 = \exp(:f_2:)\varsigma_{\rm i}, && \text{first order},\\ &\varsigma_{\rm f}^2 =: f_3 : \varsigma_{\rm f}^1, && \text{second order},\\ &\varsigma_{\rm f}^3 =: f_4 : \varsigma_{\rm f}^1 + \tfrac{1}{2} : f_3 :^2 \varsigma_{\rm f}^1, && \text{third order}.\\ &\ldots\ldots \end{aligned} \tag{12}$$

## 3. Calculation of nonlinear particle trajectories with space charge on

The electric potential generated by the space charge beam is calculated according to the two assumptions: 1) the particles distribute uniformly in the 3D ellipsoid; 2) the particles distribute in the 3D ellipsoid in Gaussian manner. In the first case, the potential is expressed as

$$\psi_s = -\frac{3IT_{\rm rf}}{8\pi\varepsilon_0\gamma_0 XYZ}(\mu_x x^2 + \mu_y y^2 + \mu_z z_{\rm r}^2), \tag{13}$$

$$\mu_x = \frac{XYZ\gamma}{2}\int_0^\infty \frac{{\rm d}\xi}{(X^2+\xi)\sqrt{(X^2+\xi)(Y^2+\xi)(Z^2\gamma^2+\xi)}},$$

$$\mu_y = \frac{XYZ\gamma}{2}\int_0^\infty \frac{{\rm d}\xi}{(Y^2+\xi)\sqrt{(X^2+\xi)(Y^2+\xi)(Z^2\gamma^2+\xi)}},$$

$$\mu_z = \frac{XYZ\gamma}{2}\int_0^\infty \frac{{\rm d}\xi}{(Z^2\gamma^2+\xi)\sqrt{(X^2+\xi)(Y^2+\xi)(Z^2\gamma^2+\xi)}}, \tag{14}$$

where $I$ is the average beam current of the pulsed beams; $T_{\rm rf}$ is the beam repetition period; $X$, $Y$ and $Z$ are the beam dimensions; $z_{\rm r}$ is the longitudinal position of the arbitrary particle relative to the position of the reference particle; $\mu_x$, $\mu_y$ and $\mu_z$ are the beam shape factors of the bunches, $\varepsilon_0$ is the dielectric constant in the vacuum.

In the second case, the potential is

$$\psi_s = \frac{IT_{\rm rf}}{8\pi^{3/2}\varepsilon_0}\int_0^\infty \frac{\exp\left[-\left(\dfrac{x^2}{2\sigma_x^2+\xi}+\dfrac{y^2}{2\sigma_y^2+\xi}+\dfrac{z_r^2\gamma_0^2}{2\sigma_z^2\gamma_0^2+\xi}\right)\right]}{\sqrt{(2\sigma_x^2+\xi)(2\sigma_y^2+\xi)(2\sigma_z^2\gamma_0^2+\xi)}}{\rm d}\xi, \tag{15}$$

where $\sigma_x$, $\sigma_y$ and $\sigma_z$ are the root mean square (RMS) pulsed beam dimensions.

To calculate the particle motion with the space charge effects, the electric potentials in Eqs. (3) and (5) each should have two parts: the applied potential and the beam self potential as shown in Eq. (13) or (15). Applying the Hamiltonian formalism and symplectic map described above to the space charge dominated beam calculations, the equations of particle motion can be solved and the second order solutions are obtained.

It is important to know that in the calculation of space charge dominated beam transport each optical element has to be divided into some small segments along the design orbit. Using the Lie map, the particle advances are calculated step by step along the design orbit.

## 4. Code performance

The steps of the code running are described as follows:

1) Generate the initial particle distribution randomly in the 3D ellipsoid.

2) Calculate the linear transport in an optical system defined by the user with the space charge off. If the system or a part of the system needs to be op-

timized, the code will perform the fitting procedures first, then calculate the linear transport based on the optimized system parameters again.

3) Calculate the nonlinear transport through the third order with the space charge off.

4) If the input beam current is zero, stop the code running. Otherwise, calculate the beam transport with the space charge forces on up to the second order.

In the steps (2) to (4) the beam diagrams in the phase space $(x, x')$, $(y, y')$, $(\nabla\phi, \nabla E)$ are displayed after each optical element. At the end of the code running, the beam envelopes are displayed.

## 5. Simulation examples

Using the code we calculate the low energy beam transport (LEBT) and the high energy beam transport (HEBT) systems of the 200 MHz RFQ accelerator built at Peking University (see Figs. 2 and 3). The LEBT consists of an Einzel lens and a Solenoid, delivering a 50 keV 30 mA deuteron beam to the RFQ cavity.

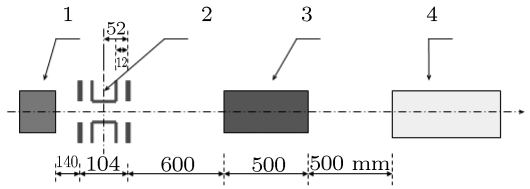



**Fig. 2.** LEBT system. 1. ion source, 2. Einzel lens, 3. solenoil, 4. RFQ cavity.

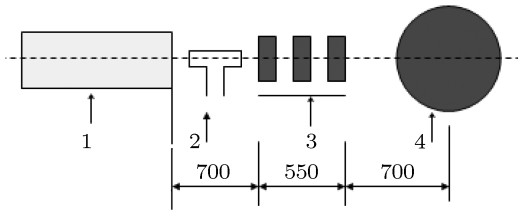



**Fig. 3.** HEBT system. 1. RFQ cavity, 2. vacuum pipe, 3. quadrupole triplet, 4. target chamber.

The HEBT consists of an quadrupole triplet, delivering a 2 MeV 25 mA deuteron beam from the RFQ cavity to the target. Because of the loss of the beam in the RFQ cavity, the beam transmission is ∼83%. The calculated results for the Gaussian distributed beam are shown in Figs.4 and 5.

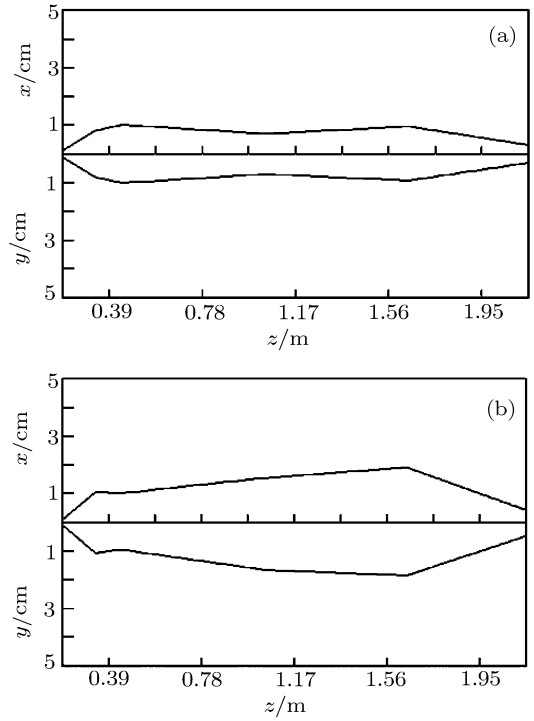



**Fig. 4.** Beam envelopes in LEBT. (a) 0 mA beam; (b) 30 mA beam.

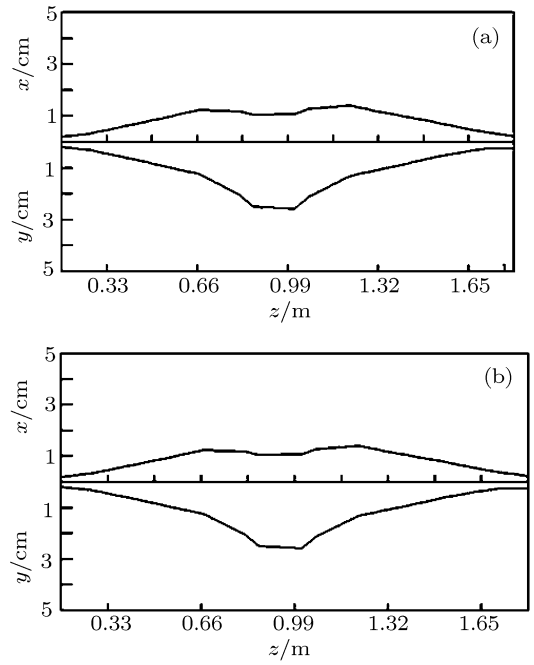



**Fig. 5.** Beam envelopes in HEBT. (a) 0 mA beam; (b) 25 mA beam.

To verify the correctness of the code, we also calculate the beam transport in the HEBT system with TRACE-3D. The results are shown in Fig.6. We can see that the beam envelopes both by LEADS-3D and TRAC-3D are very close.

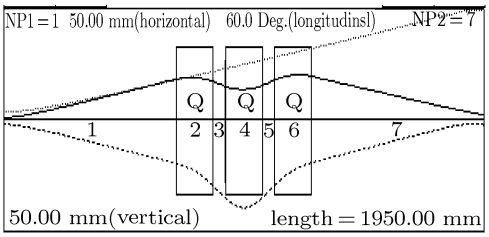



**Fig. 6.** Beam envelopes in HEBT (25 mA) (by TRACE-3D).

# 6. Conclusions

LEADS-3D is developed for intense bunched beam transport simulations in beam transport lines, high voltage electrostatic accelerators to the second order approximation. If the space charge effects are not included, it also calculates the QWR and SLR rf structures, and all of the optical elements mentioned are calculated to the third order approximation. The particle distribution in the 3D beam ellipsoid is of Gaussian or uniform type. The theoretical analysis that the code is based on is performed with the Lie algebraic method. The optical system can be optimized to achieve good configure parameters.

# References

[1] Lü J Q 1995 *Nucl. Instru. & Methods* A **355** 253
[2] Lü J Q and Quan S W 1994 *Nucl. Instru. & Methods* A **346** 31
[3] Dragt A J 1982 *AIP Conf. Proc.* **87** 147
[4] Lü J Q and Li L H 2004 *Chin. Phys.* **13** 1665
[5] Lü J Q, Li J H and Li C L 2004 *Chin. Phys.* **13** 657
[6] Lü J Q and Zhang Z 2007 *Chin. Phys.* **16** 1280
[7] Goldstein H 2002 *Classical Mechanics* 3rd Ed (California: Addison-Wesley)
[8] Dragt A J and Finn J 1976 *J. Math. Phys.* **17** 2215