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AN INVESTIGATION OF THE THERMAL-WAVE MODEL USING THE GALERKIN METHOD

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Abstract

The transverse dynamics of a charged particle beam throughout a generical device is approached here by means of the thermal wave model. A solution of the thermal-wave equation is proposed by means of the Galerkin method.

I – INTRODUCTION

The impressive analogy between electromagnetic beam optics on one side and the propagation of relativistic charged particles, in paraxial approximation, on the other side can be easily understood for the latter if we conjecture that the transverse beam profile is described by a *wave function* satisfying a *Schrödinger-type* wave equation (Thermal Wave Model) [1]. In electromagnetic wave optics the propagation of a monochromatic beam can be described starting from the Helmotz equation and introducing the so-called slowly-varying-amplitude approximation along the propagation direction. This enables us to describe the envelope of the rays (paraxial approximation) which represents the r.m.s. (spot size), over the transverse plane, of the electromagnetic energy distribution around the beam axis (Fock-Leontovich parabolic equation) [2].

Similarly, the usual description of the transfer of a relativistic charged particle beam, characterised by the longitudinal factor γ, involves a sort of *paraxial approximation* by which the transverse dynamics can be expressed in terms of an envelope of many trajectories of the beam particles. Also in this case the envelope describes a slow variation of the beam spot size along the propagation direction.

Let us consider the transverse dynamics of a relativistic charged particle beam which travels along the z-axis with uniform velocity βc ($\beta \approx 1$). It interacts with the surrounding

medium through a potential $u(\mathbf{r}_\perp, z)$ ($\mathbf{r}_\perp=(x_1, x_2)$, being x_1 and x_2 the transverse coordinates), and suffers the thermal spreading. According to the thermal wave model (TWM) [1], in the case of negligible longitudinal dynamics, transverse beam dynamics is governed by a Schrödinger-type equation for a complex wave function $\Psi(\mathbf{r}_\perp, z)$ called the beam wave function (BWF) [1]

$$i\varepsilon \frac{\partial \Psi}{\partial z} = -\frac{\varepsilon^2}{2} \nabla_\perp^2 \Psi + U(\mathbf{r}_\perp, z)\, \Psi \,, \tag{I.1}$$

where we have introduced the dimensionless potential $U(\mathbf{r}_\perp, z)$ as

$$U(\mathbf{r}_\perp, z) = \frac{u(\mathbf{r}_\perp, z)}{m_0 \gamma \beta^2 c^2} \,.$$

This dimensionless potential is a sort of effective potential as a result of the interaction of the charged particles with the surrounding medium. Usually, in the conventional accelerating machines, this potential is obtained by means of magnetic devices such as dipoles, quadrupoles, sextupoles, etc., whose typical transverse effects are focusing and defocusing of the beam as it propagates along its orbit.

In particular, in the case in which the vector potential A(x,y,z) (cartesian coordinates) is along z, the x and y component of Lorentz force on each particle are, respectively:

$$F_x = \frac{\partial}{\partial x}(q\beta cA) \equiv -\frac{\partial}{\partial x} u(x,y,z) \,,$$
$$F_y = \frac{\partial}{\partial y}(q\beta cA) \equiv -\frac{\partial}{\partial y} u(x,y,z) \,.$$

Consequantly, by using (I.1):

$$U(x,y,z) = -\frac{q}{P_0} A(x,y,z) \,,$$

where q is the particle charge and $P_0=mg\beta^2c^2$ (m being the particle rest mass). Therefore, the esplicit form of previous equation can found by giving the magnetic field $\mathbf{B} = \mathbf{B}(\mathbf{r}_\perp, z)$ generated by the device and using $\mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r}_\perp, z)$. For example, for regular multipoles, i.e. those for which the field in the plane of the machine is parallel to the main dipole field, the component $B_y(x,y,z)$ can be expanded, up to decapole, as [3]:

$$\frac{q}{P_0} B(x,y,z) = \frac{q}{P_0} B(0,0,z) + \frac{k_1(z)}{1!} x + \frac{k_2(z)}{2!} (x^2-y^2) + \\ + \frac{k_3(z)}{3!} (x^3-3xy^2) + \frac{k_4(z)}{4!} (x^4 - 6x^2y^2 + y^4) \,,$$

where for n= 1, 2, ...

$$k_n(z) \equiv \frac{q}{P_0} \left(\frac{\partial^n B_y}{\partial x^n} \right)_{(0,0,z)}$$

are the multipole strengths.

We note that equation (I.1) is homogeneous, linear, and with variable coefficients. In this equation the role of the diffraction parameter is played by the transverse emittance ε and the analogue of the time t is represented by the longitudinal co-ordinate z=ct. Bearing in mind the well-known norm conservation law for Schrödinger-like equation, we get the physical meaning of the wave function which can be related to the density of the beam. In fact, if N is the total number of particles and ρ the particle number density, we have the following relationship

$$\rho(\mathbf{r}_\perp, z) = N\, |\Psi(\mathbf{r}_\perp, z)|^2 ,$$

provided the normalisation for Ψ

$$\iint |\Psi(\mathbf{r}_\perp, z)|^2 \, d^2\mathbf{r}_\perp = 1 . \tag{I.2}$$

Hereafter we consider the special case of cylindrical symmetry. This hypothesis can be considered in the case in which the source produced an initial beam density profile with equal vertical and orizontal emittances, say $\varepsilon_x=\varepsilon_y=\varepsilon$ (round beam).So, by using the cylindrical coordinates (r, j, z) we assume:

$$U=U(r,z) , \quad \Psi=\Psi(r,z) . \tag{I.3}$$

In particular, the physical meaning of the wave-function Ψ in this symmetry will be discussed in some details in Section II. Besides we shall show that, under suitable conditions (boundary conditions and initial conditions), equation (I.1) has a unique solution in Section III, whereas in Section IV the Galerkin method to solve this partial differential equation will be proposed.

We want to underline that the initial condition implies the knowledge of the function Ψ at z=0, formally

$$\Psi(r,z=0) = \Psi_0(r) , \qquad 0 \le r \le R , \tag{I.4}$$

whereas two reasonable boundary conditions can be written in the form

$$\begin{cases} \left.\dfrac{\partial \Psi}{\partial r}\right|_{r=0} = 0 , \\ \lim\limits_{R\to\infty} \Psi\big|_{r=R} = 0 . \end{cases} \tag{I.5}$$

The first condition, essentially due to the azimuthal symmetry; implies immediately that

$$\left.\frac{\partial |\Psi|}{\partial r}\right|_{r=0} = 0 ,$$

while the second one states the distance R from the symmetry axis is the upper bound where one can find particles, namely R is the radius containing the bunch.

II – PHYSICAL INTERPRETATIONS

The physical meaning of the function Ψ can be fully revealed if one is able to write the equation for its modulus and phase. Let us put, therefore,

$$\Psi(\mathbf{r}_\perp,z) = M(\mathbf{r}_\perp,z)\, e^{i\,\varphi(\mathbf{r}_\perp,z)/\varepsilon}\,,$$

where M and φ are real functions, and let us try to find the differential equation governing M(r,z) and φ(r,z). Because

$$\frac{\partial\Psi}{\partial z} = \left(\frac{\partial M}{\partial z} + \frac{i}{\varepsilon} M \frac{\partial\varphi}{\partial z}\right) e^{i\,\varphi/\varepsilon}\,,$$
$$\nabla_\perp^2\Psi = \left\{\nabla_\perp^2 M + \frac{i}{\varepsilon}\left[\nabla_\perp\cdot(M\nabla_\perp\varphi) + \nabla_\perp M\cdot\nabla_\perp\varphi\right] - \frac{M}{\varepsilon^2}|\nabla_\perp\varphi|^2\right\} e^{i\,\varphi/\varepsilon}\,,$$

substituting in equation (I.1) and splitting the real part from the imaginary one, it is

$$\begin{cases}\dfrac{\partial M}{\partial z} = -\dfrac{1}{2}\nabla_\perp\cdot(M\nabla_\perp\varphi) - \dfrac{1}{2}\nabla_\perp M\cdot\nabla_\perp\varphi\,,\\[2ex] M\dfrac{\partial\varphi}{\partial z} = \dfrac{\varepsilon^2}{2}\nabla_\perp^2 M - \dfrac{M}{2}|\nabla_\perp\varphi|^2 - U\,M\,.\end{cases} \qquad \text{(II.1)}$$

The first partial differential equation of the system (II.1) can be rearranged as follows

$$M\frac{\partial M}{\partial z} = -\frac{M}{2}\nabla_\perp\cdot(M\nabla_\perp\varphi) - \frac{M}{2}\nabla_\perp M\cdot\nabla_\perp\varphi\,,$$

or using a vector identity [5]

$$\frac{\partial M^2}{\partial z} + \nabla_\perp\cdot\left(M^2\,\nabla\varphi\right) = 0\,.$$

Introducing the vector field

$$\mathbf{u}(r,z) \equiv \nabla_\perp\varphi(r,z)\,, \qquad \text{(II.2)}$$

the last equation is easily rewritten as

$$\frac{\partial M^2}{\partial z} + \nabla_\perp\cdot(M^2\,\mathbf{u}) = 0\,. \qquad \text{(II.3)}$$

Equation (II.2) can be interpretated as a *continuity* equation.

On the contrary the second equation of the system (II.1) can be rearranged as follows

$$\frac{\partial\varphi}{\partial z} = \frac{\varepsilon^2}{2\,M}\nabla_\perp^2 M - \frac{1}{2}|\nabla_\perp\varphi|^2 - U\,.$$

If we take the transverse gradient on both side of this equation and we remember the definition (II.2), we have

$$\frac{\partial\mathbf{u}}{\partial z} + \frac{1}{2}\nabla_\perp u^2 = \frac{\varepsilon^2}{2}\nabla_\perp\left(\frac{1}{M}\nabla_\perp^2 M\right) - \nabla_\perp U\,,$$

namely, using the convective derivative [5]

$$\frac{d}{dz} = \frac{\partial}{\partial z} + \mathbf{v} \cdot \nabla_\perp$$

we can finally write

$$\frac{du}{dz} = \frac{\varepsilon^2}{2} \nabla_\perp \left(\frac{1}{M} \nabla_\perp^2 M \right) - \nabla_\perp U \, . \tag{II.4}$$

This equation can be interpreted as the balance momentum equation where the forcing term can be imagined composed by a pressure term

$$P = \frac{\varepsilon^2}{2\,M} \nabla_\perp^2 M$$

and by the conservative potential term U. We point out that M describes the density profile and it is related to the macroscopic transverse velocity field by means of equation (II.2): the macroscopic transverse velocity is a conservative field and φ is its scalar potential.

We observe that the results of this Section are independent of the particular symmetry choosen.

In order to solve equation (I.1) we have to assign the initial and boundary conditions. The boundary conditions are already known and homogeneous, whereas the initial conditions of the BWF depend on the initial beam configuration in terms of number density and macroscopic transverse velocity field. The initial value of the modulus Ψ is given by the particle number density, and initial value of the phase is related to the transverse velocity field. We immediately assume that the phase is defined unless than a constant which doesn't produce any effect.

III – UNIQUENESS OF THE SOLUTION

The first task we have to do is to prove that the solution of equation (I.1) with initial condition (I.4) and boundary conditions (I.5) is unique. In fact, let imagine that two solutions of this problem can exist: we call them Ψ_1 and Ψ_2. Because of the linearity of the problem, one can introduce a new solution defined as the following difference

$$\Delta\Psi = \Psi_1 - \Psi_2 \, , \tag{III.1}$$

which is a new solution of differential equation (I.1). Formally one can say that this new function has to satisfy the differential equation

$$i\varepsilon \frac{\partial(\Delta\Psi)}{\partial z} = -\frac{\varepsilon^2}{2} \nabla_\perp^2 (\Delta\Psi) + U\,\Delta\Psi \, , \tag{III.2}$$

with the homogeneous initial condition

$$\Delta\Psi(r, z=0) = 0 \, , \qquad 0 \le r \le R \, , \tag{III.3}$$

and boundary conditions

$$\begin{cases} \left.\dfrac{\partial(\Delta\Psi)}{\partial r}\right|_{r=0} = 0 , \\ \lim\limits_{R\to\infty} \Delta\Psi|_{r=R} = 0 . \end{cases} \tag{III.4}$$

Multiplying both sides of equation (III.2) for the conjugate of $\Delta\Psi$, it is

$$i\varepsilon\,(\Delta\Psi)^{*}\,\frac{\partial(\Delta\Psi)}{\partial z} = -\,\frac{\varepsilon^2}{2}\,(\Delta\Psi)^{*}\nabla_{\perp}^{2}(\Delta\Psi) + U\,|\Delta\Psi|^2 . \tag{III.5}$$

The vector identity [5]

$$\nabla_{\perp}\cdot\left[(\Delta\Psi)^{*}\nabla_{\perp}(\Delta\Psi)\right] = \nabla_{\perp}(\Delta\Psi)\cdot\,\nabla_{\perp}(\Delta\Psi)^{*} + (\Delta\Psi)^{*}\nabla_{\perp}^{2}(\Delta\Psi)$$

enables us to rewrite equation (III.5) in the equivalent form

$$\frac{i\varepsilon}{2}\frac{\partial|\Delta\Psi|^2}{\partial z} = -\,\frac{\varepsilon^2}{2}\left\{\nabla_{\perp}\cdot\left[(\Delta\Psi)^{*}\nabla_{\perp}(\Delta\Psi)\right] - |\nabla_{\perp}(\Delta\Psi)|^2\right\} + U\,|\Delta\Psi|^2 . \tag{III.6}$$

We have to integrate equation (III.6) all over the range (0,R). Because of the boundary condition (III.4), it is

$$\int_0^R r\,\nabla_{\perp}\cdot\left[(\Delta\Psi)^{*}\nabla_{\perp}(\Delta\Psi)\right]dr = \int_0^R r\,\frac{\partial}{\partial r}\left[(\Delta\Psi)^{*}\nabla_{\perp}(\Delta\Psi)\right]dr =$$

$$\int_0^R \frac{\partial}{\partial r}\left[r\,(\Delta\Psi)^{*}\nabla_{\perp}(\Delta\Psi)\right]dr = r\,(\Delta\Psi)^{*}\nabla_{\perp}(\Delta\Psi)\Big|_{r=R} - r\,(\Delta\Psi)^{*}\nabla_{\perp}(\Delta\Psi)\Big|_{r=0} = 0 ,$$

and we can conclude

$$\frac{i\varepsilon}{2}\frac{d}{dz}\int_0^R r\,|\Delta\Psi|^2\,dr = \frac{\varepsilon^2}{2}\int_0^R r\,|\nabla_{\perp}(\Delta\Psi)|^2\,dr + \int_0^R r\,U\,|\Delta\Psi|^2\,dr . \tag{III.7}$$

The left side of equation (III.7) is an imaginary quantity, whereas the right one is a non negative, real number; they have to be simultaneously zero, and therefore

$$\frac{d}{dz}\int_0^R r\,|\Delta\Psi|^2\,dr = 0 . \tag{III.8}$$

From equation (III.8) it follows at once

$$\int_0^R r\,|\Delta\Psi|^2\,dr = \text{constant with } z , \tag{III.9}$$

where the constant has to be zero for (III.3). Thus we can conclude that in (III.9) the integrand function has to be zero, and that

$$|\Delta\Psi| = 0 \;\Rightarrow\; \mathrm{Re}(\Delta\Psi) = \mathrm{Im}(\Delta\Psi) = 0 \,.$$

This implies immediately that $\Psi_1 = \Psi_2$, namely the solution is unique.

IV – THE GALERKIN METHOD

It is very hard to find the solution of partial differential equation (I.1) for a generical potential function U. Particular solutions have been found [4] in the case of symmetrical geometries and for a polynomials expansion for U. In this Section we propose a general way to find an approximate solution of this problem by means of the Galerkin method [6]. We start with the trial function

$$\Psi_N = \sum_{i=1}^{N} a_i(z)\, w_i(r)\,, \qquad \text{(IV.1)}$$

with $w_i(r)$ real known basis function of compact support, and $a_i(z)$ complex and unknown function describing the *time* evolution of the system. Formally

$$w_i(r) \in \mathbf{R}\,,\; a_i(z) \in \mathbf{C}\,,\; \forall i = 1, \cdots, N\,.$$

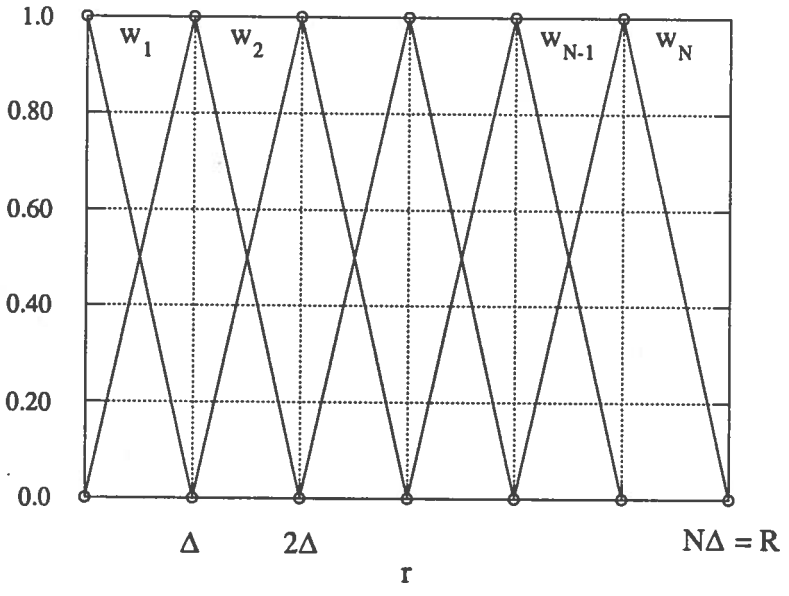

Figure 1 – Expansion basis.

The basis functions we want to use for numerical simulations are the piece-wise linear functions (namely triangular pulses) shown in Figure 1, defined as

$$w_1 = \begin{cases} 1 - r/\Delta & 0 \le r \le \Delta \,, \\ 0 & \text{otherwise} \,, \end{cases} \tag{IV.2}$$

and for i = 2, 3, ... , N it is

$$w_i = \begin{cases} 2 - i + r/\Delta & (i-2)\Delta \le r \le (i-1)\Delta \,, \\ i - r/\Delta & (i-1)\Delta \le r \le i\Delta \,, \\ 0 & \text{otherwise} \,. \end{cases} \tag{IV.3}$$

The set of all piece-wise linear functions in (0,R) is dense in $L^2(0,R)$. The derivative with respect to the radial co-ordinate r (we shall indicate with the dot for shortness) are given by

$$\dot{w}_1 = \begin{cases} -1/\Delta & 0 \le r \le \Delta \,, \\ 0 & \text{otherwise} \,, \end{cases} \tag{IV.4}$$

and for i = 2, 3, ... , N it is

$$\dot{w}_i = \begin{cases} 1/\Delta & (i-2)\Delta \le r \le (i-1)\Delta \,, \\ -1/\Delta & (i-1)\Delta \le r \le i\Delta \,, \\ 0 & \text{otherwise} \,. \end{cases} \tag{IV.5}$$

We want only to underline that, for the particular choice for the basis functions discussed, all the $w_i(r)$ vanishe for r=R, that is $w_i(R)=0$.

Substituting the proposed expansion (IV.1) in (I.1), it is

$$i\varepsilon \sum_{i=1}^{N} \frac{da_i}{dz} w_i = -\frac{\varepsilon^2}{2} \sum_{i=1}^{N} a_i \frac{1}{r} \frac{d}{dr}\left(r \frac{dw_i}{dr}\right) + U \sum_{i=1}^{N} a_i w_i \,. \tag{IV.6}$$

Making the projection of equation (IV.6) onto the functional space described by the basis functions, with the inner product defined as

$$\langle f(r), g(r) \rangle \equiv \int_0^R r\, f(r)\, g(r)\, dr \,,$$

one can affirme that

$$i\varepsilon \sum_{i=1}^{N} \frac{da_i}{dz} \langle w_i, w_j \rangle = -\frac{\varepsilon^2}{2} \sum_{i=1}^{N} a_i \left\langle \frac{1}{r} \frac{d}{dr}\left(r \frac{dw_i}{dr}\right), w_j \right\rangle + U \sum_{i=1}^{N} a_i \langle w_i, w_j \rangle \,. \tag{IV.7}$$

Now, an integration by parts enables us to write

$$\left\langle \frac{1}{r} \frac{d}{dr}\left(r \frac{dw_i}{dr}\right), w_j \right\rangle = r\, w_j\, \dot{w}_i\big|_{r=R} - r\, w_j\, \dot{w}_i\big|_{r=R} - \langle \dot{w}_i, \dot{w}_j \rangle = -\langle \dot{w}_i, \dot{w}_j \rangle \,. \tag{IV.8}$$

Thus, using the notations

$$A_{ij} = A_{ji} = \langle w_i, w_j \rangle = \int_0^R r\, w_i(r)\, w_j(r)\, dr\,,$$

$$L_{ij} = L_{ji} = -\langle \dot{w}_i, \dot{w}_j \rangle = -\int_0^R r\, \dot{w}_i(r)\, \dot{w}_j(r)\, dr\,, \qquad \text{(IV.9)}$$

$$V_{ij}(z) = V_{ji}(z) = \langle w_i\sqrt{U}, w_j\sqrt{U} \rangle = \int_0^R r\, U(r,z)\, w_i(r)\, w_j(r)\, dr\,,$$

and introducing the unknown vector[1]

$$\mathbf{a} \equiv (a_1, \cdots, a_N)^T\,,$$

equation (IV.7) can be written in the matrix form by means of (IV.8)

$$i\varepsilon\, \mathbf{A}\frac{d\mathbf{a}}{dz} + \frac{\varepsilon^2}{2}\mathbb{L}\,\mathbf{a} - \mathbb{V}\,\mathbf{a} = 0\,,$$

or as the initial values problem

$$\begin{cases} \dfrac{d\mathbf{a}}{dz} = \dfrac{i}{\varepsilon}\mathbf{A}^{-1}\left[\dfrac{\varepsilon^2}{2}\mathbb{L} - \mathbb{V}\right]\mathbf{a}\,, \\ \mathbf{a}(0) = \mathbf{a}_0\,. \end{cases} \qquad \text{(IV.9)}$$

The matices A and L are computed in the Appendix A, whereas details about the initial condition $\mathbf{a}_0$ are given in the Appendix B.

All the properties of the approximate solution (IV.1) are written in the system (IV.9), which is a first order differential equations system. The solution of this system could be found in a closed form, but it is easier to solve numerically by means the fourth-order Runge-Kutta method, for example. Its properties are defined by the properties of the matrices:

A a real, symmetric and banded matrix, defined positive;
L a real, symmetric and banded matrix, defined negative;
V a symmetric, banded matrix.

Explicit calculations cannot be performed for the matrix V, whose elemets depend upon the selected (quadrupole, sextupole, octupole) potential U.

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[1] In this paper the vectors will be indicated by lowercase and bold letter (**p**), whereas the matrix by an uppercase and outline letter (𝕂).

IV – CONCLUSIONS AND PERSPECTIVES

In this note, in order to find a numerical solution of a Schrödinger-like equation, within the framework of TWM [1], we propose to use Galerkin method. It is shown that the partial differential equation describing the model can be rewritten as a system of ordinary differential equations which can be solved in a robust way by using, for example, a fourth-order Runge-Kutta method.

We hope, in a near future, to perform numerical calculations in order to study the non-linear transverse dynamics of a bunch, interacting with a device made of quadrupole with sextupole and octupole deviations, or, more generally, with a given profile of magnetic field.

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APPENDIX A

In this appendix we have to compute the matrices A and $\mathbb{L}$, defined by (IV.9). These matrices are symmetric and banded, and the non-vanishing elements are [4]

$$\begin{cases} A_{11} = \frac{\Delta^2}{12}, \; A_{12} = \frac{\Delta^2}{12}, \\ A_{i,i-1} = \frac{\Delta^2}{12}, \; A_{i,i} = \frac{2\Delta^2(i-1)}{3}, \; A_{i,i+1} = \frac{\Delta^2}{12}, \quad (i=2,\ldots,N-1), \\ A_{N,N-1} = \frac{\Delta^2}{12}, \; A_{N,N} = \frac{2\Delta^2(i-1)}{3}; \end{cases} \tag{A.1}$$

$$\begin{cases} L_{11} = -\frac{1}{2}, \; L_{12} = \frac{1}{2}, \\ L_{i,i-1} = i - \frac{3}{2}, \; L_{i,i} = 2 - 2i, \; L_{i,i+1} = i - \frac{1}{2}, \quad (i=2,\ldots,N-1), \\ L_{N,N-1} = N - \frac{3}{2}, \; L_{N,N} = 2 - 2N. \end{cases} \tag{A.2}$$

APPENDIX B

To compute the initial condition $\mathbf{a}_0$ one has to know the initial transverse ditribution of the beam; this implies that one has to do a choice, and thus the calculations are not general. But a particular initial transverse distribution of the beam which is commonly used in all the simulations code,. is the gaussian distribution, namely the initial transverse condition

$$\Psi(r,0) = \Psi_0(r) = \frac{1}{\sigma\sqrt{\pi}} e^{-0.5\,(r/\sigma)^2}\,, \tag{B.1}$$

verifying [4] the normalisation condition (I.2).

The knowledge of the initial distribution can be used to compute the initial value of the vector **a**, that is

$$\Psi(r,0) = \sum_{i=1}^{N} a_i(0)\, w_i(r)\,, \tag{B.2}$$

or projecting onto the base functions space, we obtain [4]

$$b_j = \langle \Psi(r,0), w_j(r) \rangle = \sum_{i=1}^{N} \langle w_j(r), w_i(r) \rangle\, a_i(0) = \sum_{i=1}^{N} A_{ij}\, a_i(0)\,. \tag{B.3}$$

In a matrix form, to obtain tha values $a_i(0)$, one has to invert the matrix **A** (computed in Appendix A), formally

$$\mathbf{a}(0) = \mathbf{A}^{-1}\,\mathbf{b}\,.$$

The vector **b** is easily computed [4] observing that

$$r\,\Psi(r,0) = \frac{r}{\sigma\sqrt{\pi}} e^{-0.5\,(r/\sigma)^2} = -\frac{\sigma}{\sqrt{\pi}} \frac{d}{dr} e^{-0.5\,(r/\sigma)^2}\,,$$

and therefore performing the integration (j=2, 3, ..., N)

$$\begin{aligned} b_1 &= \int_0^{\Delta} r\,\Psi(r,0)\, w_1(r)\, dr = \frac{1}{\sqrt{\pi}} - \frac{\sigma}{\Delta\sqrt{2}}\, \Phi\left(\frac{\Delta}{\sigma\sqrt{2}}\right), \\ b_j &= \int_0^{\Delta} r\,\Psi(r,0)\, w_j(r)\, dr = \frac{\sigma}{\Delta\sqrt{2}} \left\{ 2\Phi\left[\frac{(j-1)\Delta}{\sigma\sqrt{2}}\right] - \Phi\left[\frac{(j-2)\Delta}{\sigma\sqrt{2}}\right] - \Phi\left(\frac{j\Delta}{\sigma\sqrt{2}}\right) \right\}. \end{aligned} \tag{B.4}$$

The function F(x) is the error function defined as [4]

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt\,.$$