Appendix **A**

Preparing wavepackets

A realistic time-dependent simulation of any physical system requires more than just an algorithm to perform the time evolution. The spatial dependence of the EM fields must be either specified at the initial time instance or by means of a current source. For various purposes a localized EM field moving in a specific direction with a particular energy is very useful. We will discuss two methods that prepare such wavepackets in one- two- and three dimensions. The first method is based on an expansion of a wavepacket in plane-waves [94], the second expands the wave-function in eigenmodes of a cavity. It turns out that the first method is much faster and can also generate non-linear polarizations, but is limited to wavepackets with a Gaussian distribution of the k-vector; the second method is slower but does not has this limitation.

A.1 Expansion in plane-waves

The electromagnetic components of a linearly polarized plane wave are [2]

$$\mathbf{E}(\mathbf{r},t) = \hat{\mathbf{e}}_1 E_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}, \tag{A.1a}$$

$$\mathbf{B}(\mathbf{r},t) = \hat{\mathbf{e}}_2 B_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}, \tag{A.1b}$$

with $\hat{\mathbf{e}}_i = \mathbf{e}_i/|\mathbf{e}_i|$. From the Maxwell Equations, it follows that the set of vectors $(\mathbf{k}, \mathbf{e}_1, \mathbf{e}_2)$ are mutually orthogonal, and related by

$$\hat{\mathbf{e}}_2 B_0 = \sqrt{\mu\varepsilon}\ \hat{\mathbf{k}} \times \hat{\mathbf{e}}_1 E_0, \tag{A.2}$$

where $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$. Making use of the orthogonality, we have for the amplitudes $E_0/B_0 = c$. Any linear combination of plane waves described by Eq. (A.1) also satisfies the Maxwell Equations. Hence, it should be possible to construct a localized wavepacket by using a linear superposition of plane waves where the wave-vectors $\mathbf{k}$ form a Gaussian function, due to the fact that the Fourier transform of a Gaussian function in k-space is a Gaussian function in real space.

The basic procedure is then this: we choose a suitable Gaussian function for the wave-vectors $\mathbf{k}$ and then integrate the plane-waves over $\mathbf{k}$. We should end up with a localized wavepacket that propagates according to our distribution in k-space. The electromagnetic fields at $t = 0$ are given, eliminating $\mathbf{e}_2$, by a linear superposition of plane waves

$$\mathbf{E}(\mathbf{r}) = E_0 \int_V d\mathbf{k}\ g(\mathbf{k}) \frac{\mathbf{e}_1}{|\mathbf{e}_1|} e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{A.3a}$$

$$\mathbf{B}(\mathbf{r}) = B_0 \int_V d\mathbf{k}\ g(\mathbf{k}) \frac{\mathbf{k}\times\mathbf{e}_1}{|\mathbf{k}|\ |\mathbf{e}_1|}\ e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{A.3b}$$

The orthogonality constraint $\mathbf{k}\cdot\mathbf{e}_1 = 0$ is satisfied if we choose $\mathbf{e}_1 = (e_y k_y - e_z k_z, e_y k_x, e_z k_x)^T$, and we are free to choose $\mathbf{e}_1$ as we like. Some of the explicit k dependence in Eq. (A.3) can then be moved outside the integral by using the identities

$$k_j\, e^{i\mathbf{kr}} = -i\frac{\partial}{\partial r_j} e^{i\mathbf{kr}}, \tag{A.4a}$$

$$k_j k_l\, e^{i\mathbf{kr}} = -\frac{\partial}{\partial r_j}\frac{\partial}{\partial r_l} e^{i\mathbf{kr}}. \tag{A.4b}$$

We choose for the k distribution the Gaussian function

$$g(\mathbf{k}) = |\mathbf{e}_1| \exp\{-(k_x - k_0)^2\sigma_x^2 - k_y^2\sigma_y^2 - k_z^2\sigma_z^2\}, \tag{A.5}$$

and at the same time make sure that the factor $1/|\mathbf{e}_1|$ cancels in the integrand. The resulting wavepacket has a spatial distribution with width $\vec{\sigma}$ and propagates with wave vector $(k_0, 0, 0)^T$.

The integrals that remain to be evaluated are

$$\mathbf{E}(\mathbf{r}) = iE_0 \begin{pmatrix} e_y\frac{\partial}{\partial y} + e_z\frac{\partial}{\partial z} \\ -e_y\frac{\partial}{\partial x} \\ -e_z\frac{\partial}{\partial x} \end{pmatrix} \int_V d\mathbf{k}\; e^{-(k_x-k_0)^2\sigma_x^2 - k_y^2\sigma_y^2 - k_z^2\sigma_z^2} e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{A.6a}$$

$$\mathbf{B}(\mathbf{r}) = B_0 \begin{pmatrix} -e_z\frac{\partial}{\partial y}\frac{\partial}{\partial x} + e_y\frac{\partial}{\partial z}\frac{\partial}{\partial x} \\ e_y\frac{\partial}{\partial z}\frac{\partial}{\partial y} + e_z\frac{\partial^2}{\partial^2 z} + e_z\frac{\partial^2}{\partial^2 x} \\ -e_y\frac{\partial^2}{\partial^2 x} - e_y\frac{\partial^2}{\partial^2 y} - e_z\frac{\partial}{\partial z}\frac{\partial}{\partial y} \end{pmatrix} \int_V d\mathbf{k}\; \frac{1}{|\mathbf{k}|} e^{-(k_x-k_0)^2\sigma_x^2 - k_y^2\sigma_y^2 - k_z^2\sigma_z^2} e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{A.6b}$$

The integral for the electric field can be solved analytically, yielding

$$\int_V d\mathbf{k}\; e^{-(k_x-k_0)^2\sigma_x^2 - k_y^2\sigma_y^2 - k_z^2\sigma_z^2} e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ik_0 x} f_E(x) f_E(y) f_E(z), \tag{A.7}$$

where

$$f_E(x) = \frac{\sqrt{\pi}}{\sigma_x} \exp\left(-\frac{x^2}{4\sigma_x^2}\right), \tag{A.8}$$

and similar expressions hold for $f_E(y)$ and $f_E(z)$. The individual electric field components can now be obtained by differentiation. Unfortunately, the integral for the magnetic field is somewhat more difficult due to the coupling of all k components by the presence of the factor $1/|\mathbf{k}|$. This factor can be removed by introducing another variable, over which must then be integrated:

$$\frac{1}{|\mathbf{k}|} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du e^{-u^2|\mathbf{k}|^2}. \tag{A.9}$$

The integral for the magnetic field now decouples and the k-space integral can be evaluated:

$$I_B = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du \int_V d\mathbf{k}\; e^{-u^2|\mathbf{k}|^2} e^{-(k_x-k_0)^2\sigma_x^2 - k_y^2\sigma_y^2 - k_z^2\sigma_z^2} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{A.10}$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du \exp\left\{\frac{ik_0 x\sigma_x^2 - k_0^2\sigma_x^2 u^2}{\sigma_x^2 - u^2}\right\} f_B(x,u) f_B(y,u) f_B(z,u), \tag{A.11}$$

where

$$f_B(x,u) = \frac{\sqrt{\pi}}{\sqrt{\sigma_x^2 + u^2}} \exp\left(-\frac{x^2}{4\sigma_x^2 + u^2}\right), \tag{A.12}$$

and similar expressions for $f_B(y,u)$ and $f_E(z,u)$. The integral over u remains, and must be computed numerically. Summarizing, we have the following expressions for the electromagnetic fields:

$$\mathbf{E}(\mathbf{r}) = iE_0 \begin{pmatrix} e_y\frac{\partial}{\partial y} + e_z\frac{\partial}{\partial z} \\ -e_y\frac{\partial}{\partial x} \\ -e_z\frac{\partial}{\partial x} \end{pmatrix} e^{ik_0 x} f_E(x) f_E(y) f_E(z) \tag{A.13a}$$

$$\mathbf{B}(\mathbf{r}) = B_0 \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du \begin{pmatrix} -e_z\frac{\partial}{\partial y}\frac{\partial}{\partial x} + e_y\frac{\partial}{\partial z}\frac{\partial}{\partial x} \\ e_y\frac{\partial}{\partial z}\frac{\partial}{\partial y} + e_z\frac{\partial^2}{\partial^2 z} + e_z\frac{\partial^2}{\partial^2 x} \\ -e_y\frac{\partial^2}{\partial^2 x} - e_y\frac{\partial^2}{\partial^2 y} - e_z\frac{\partial}{\partial z}\frac{\partial}{\partial y} \end{pmatrix} \times$$
$$\exp\left\{\frac{ik_0 x\sigma_x^2 - k_0^2\sigma_x^2 u^2}{\sigma_x^2 - u^2}\right\} f_B(x,u) f_B(y,u) f_B(z,u) \tag{A.13b}$$

The actual physical fields can be obtained by taking the real parts of the above equations. Reduction to two dimensions can be achieved by assuming that the partial derivative with respect to the z-coordinate is zero for all the fields, and $f_E(z) = f_B(z,u) = 1$. For reduction to one dimension we additionally assume that the partial derivative with respect to the y-coordinate is zero for all the fields and $f_E(y) = f_B(y,u) = 1$.

A.1.1 Circular and elliptic polarized waves

Up to now, the amplitudes E_0 and B_0 were considered to be real, and the EM wave linearly (and orthogonal) polarized. In general, both the EM fields can be a linear superposition of fields oriented in the $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ direction [2]:

$$\mathbf{E}(\mathbf{r}) = \int_V d\mathbf{k}\; g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \left(\hat{\mathbf{e}}_1 E_0 + \hat{\mathbf{e}}_2 E_0'\right), \tag{A.14a}$$

$$\mathbf{B}(\mathbf{r}) = \sqrt{\mu\varepsilon} \int_V d\mathbf{k}\; g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \left(\hat{\mathbf{e}}_2 E_0 - \hat{\mathbf{e}}_1 E_0'\right). \tag{A.14b}$$

It is convenient to express the amplitudes E_0 and E_0' as a complex number (we obtain the resulting fields by taking the real part),

$$E_0 = |E_0| e^{i\phi}, \tag{A.15a}$$

$$E_0' = |E_0'| e^{i\phi'}. \tag{A.15b}$$

In the special case that the phases ϕ and ϕ' are equal, the wave is said to be linearly polarized. The polarization angle, the angle between the vectors $\hat{\mathbf{e}}_1 E_0$ and $\hat{\mathbf{e}}_2 E_0'$, is then given by $\theta = \arctan(E_0'/E_0)$. In the previous section, we assumed $E_0' = 0$, and hence the polarization angle was 90 degrees. If the phases ϕ and ϕ' are not equal, the wave is said to be elliptically polarized [2]. In the special case that the phase difference is 90 degrees, and the amplitudes E_0 and E_0' are equal, there is circular polarization. For a fixed point in

space, the polarization vector will now rotate around the propagation axis with an angular frequency ω.

The procedure to construct localized wavepackets for circular and/or elliptical polarized waves is very similar to the linear case. Eliminating vector $\hat{\mathbf{e}}_2$, the fields become, in terms of the unnormalized vectors $\mathbf{e}_1$ and $\mathbf{k}$,

$$\mathbf{E}(\mathbf{r}) = E_0 \int_V d\mathbf{k}\; g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\mathbf{e}_1}{|\mathbf{e}_1|} + E_0' \int_V d\mathbf{k}\; g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\mathbf{k}\times\mathbf{e}_1}{|\mathbf{k}|\;|\mathbf{e}_1|}, \tag{A.16a}$$

$$\mathbf{B}(\mathbf{r}) = \sqrt{\mu\varepsilon} E_0 \int_V d\mathbf{k}\; g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\mathbf{k}\times\mathbf{e}_1}{|\mathbf{k}|\;|\mathbf{e}_1|} - \sqrt{\mu\varepsilon} E_0' \int_V d\mathbf{k}\; g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \frac{\mathbf{e}_1}{|\mathbf{e}_1|}. \tag{A.16b}$$

In these expressions, two different integrals occur with different prefactors, but both integrals are exactly the same as the ones occurring in the previous section. Hence, the integral without the factor $1/|\mathbf{k}|$ can be solved analtyically (cf. Eq. (A.7)), the other one must be solved numerically (cf. Eq. (A.11)).

A.2 Expansion in eigenmodes of a cavity

All wavepackets are prepared in vacuum, in which case all the EM fields must obey the wave-equation Eq. (2.5),

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2} f(\mathbf{r},t) = \nabla^2 f(\mathbf{r},t). \tag{A.17}$$

The solution of the wave equation obviously yields plane waves. However, in the direction perpendicular to the direction of propagation, the wave extends infinitely, and the systems we model are only finitely sized. The localization of the wavepacket, while satisfying the TDME, proves to be the major difficulty (and we will deal with this problem in each dimension separately). Ideally, we want the spatial and temporal dependence of one or more of the EM fields to equal a reference function, i.e. a localized wavepacket moving in a particular direction. To accomplish this, one must very carefully choose the spatial distribution of all the EM fields at the initial time instance. Since the boundary conditions and the TDME themselves must be satisfied, there is only a limited number of degrees of freedom, and certainly not all reference functions are solutions of the TDME. However, in practice, a wavepacket that does not diverge too rapidly is sufficient for most scattering problems.

One approach is to demand that one of the EM fields and the time derivative of that EM field equals the reference solution. By expansion of this EM field in eigenmodes of the cavity itself, the other EM fields can be reconstructed and the TDME are automatically satisfied.

A.2.1 One Dimension

In one dimension, the TDME for the TM-mode in vacuum reduce to the form (see Eqs. (2.51a) and (2.51b))

$$\frac{1}{c}\frac{\partial}{\partial t} E_z(x,t) = \frac{\partial}{\partial x} H_y(x,t), \tag{A.18a}$$

$$\frac{1}{c}\frac{\partial}{\partial t} H_y(x,t) = \frac{\partial}{\partial x} E_z(x,t). \tag{A.18b}$$

If we choose $E_z(x,t) = f(x-ct)$ then $H_y(x,t) = -f(x-ct)$ is a solution of these set of equations. We are free to choose any localized function for $f(x-ct)$, for example Gaussian shaped:

$$f(x,t) = \exp\left[-(x-ct-x_0)^2/\sigma^2\right]. \tag{A.19}$$

This solves the problem of the preparation of the initial wavepacket in 1D. However, in some cases, we need to know the solution of time evolution of the fields for all times, for example in the case that we want to measure the accuracy of a particular algorithm. The results generated by the algorithm can then be compared with the analytical solution. After the wavepacket hits the boundary, the function $f(x,t)$ from Eq. (A.19) will no longer describe the EM fields. A valid solution for all times can be found by expanding $f(x,t)$ in (TM-mode) eigenmodes of the cavity, which are

$$E_z(x,t) = \sum_{n=1}^{\infty} \sin(k_n x)[a_n \sin(\omega_n t) + b_n \cos(\omega_n t)], \tag{A.20a}$$

$$H_y(x,t) = -\frac{1}{2}a_0 - \sum_{n=1}^{\infty} \cos(k_n x)[a_n \cos(\omega_n t) - b_n \sin(\omega_n t)], \tag{A.20b}$$

where $k_n = n\pi/L$ and $w_n = k_n c$. At $t = 0$ we arbitrarily choose E_z to equal the reference solution. The expansion coefficients are given by the inner products with the eigenmodes:

$$a_n = \frac{2}{\omega_n L}\int_0^L dx \sin(k_n x)\frac{\partial}{\partial t} f(x,t)|_{t=0} = \frac{2\sigma\sqrt{\pi}}{L}\exp(-k_n^2\sigma^2/4)\cos(k_n x_0), \tag{A.21}$$

$$b_n = \frac{2}{L}\int_0^L dx \sin(k_n x) f(x,t=0) = \frac{2\sigma\sqrt{\pi}}{L}\exp(-k_n^2\sigma^2/4)\sin(k_n x_0). \tag{A.22}$$

After substitution of these coefficients into equation (A.20), the resulting expression for the EM fields can be simplified by application of the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} f(n)e^{2\pi i n m}dn. \tag{A.23}$$

We then find

$$E_z(x,t) = \sum_{n=-\infty}^{\infty}\left\{e^{-(2nL+x+x_0+ct)^2/\sigma^2} - e^{-(2nL+x-x_0-ct)^2/\sigma^2}\right\}, \tag{A.24a}$$

$$H_y(x,t) = -\sum_{n=-\infty}^{\infty}\left\{e^{-(2nL+x+x_0+ct)^2/\sigma^2} + e^{-(2nL+x-x_0-ct)^2/\sigma^2}\right\}. \tag{A.24b}$$

For an example of a wavepacket in one dimension see figure A-1.

A.2.2 Two Dimensions

The procedure for preparing a wavepacket in 2D is essentially analogous to the 1D case. However, it is easy to show that a localized wavepacket moving in a specific direction is not a solution of the wave-equation. If we insert the reference function

$$f(x,y,t) = f_1(y)f_2(x-ct) \tag{A.25}$$

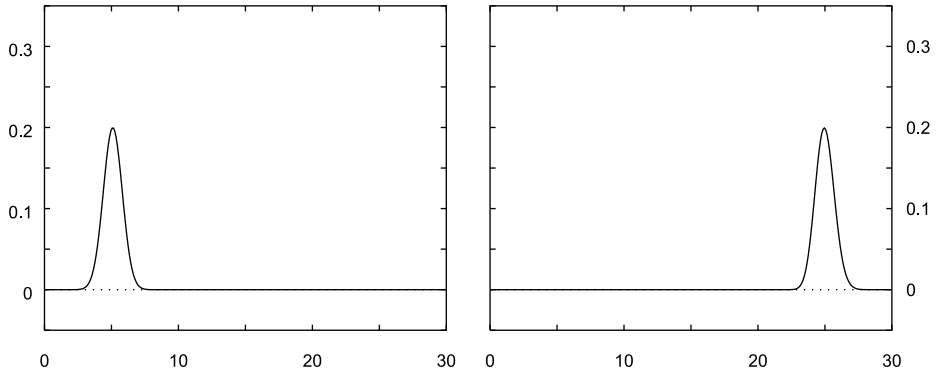

Figure A-1: Example of a wavepacket in one dimension. The cavity measures $L = 30$, with a mesh $\delta = 0.1$. Left: initial wavepacket, magnetic field intensity of a Gaussian packet with parameters $\sigma = 1$ and $x_0 = 5$. Right: magnetic field intensity distribution at $t = 20$, the time evolution is solved with the Chebyshev algorithm ($\kappa = 10^{-13}$).

into the 2D wave-equation

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2} f(x,y,t) = \nabla^2 f(x,y,t), \tag{A.26}$$

it follows that

$$f_2(x-ct)\frac{\partial^2}{\partial y^2} f_1(y) = 0, \tag{A.27}$$

and thus $f_1(y) = ay + b$, a non-localized function. Consequently, there is no initial EM field distribution that will produce a non diverging wavepacket. Nevertheless, if the divergence is not too rapid, many scattering phenomena can be simulated. We therefore choose as reference function

$$f(x,y,t) = \sin(k(x - x_0 - ct)) \exp[-((x - x_0 - ct)/\sigma_x)^{10} - ((y - y_0)/\sigma_y)^2] \tag{A.28}$$

for the TM-mode E_z field, knowing it does not satisfy the wave-equation and therefore will diverge. The wavepacket propagates in the $+x$ direction and is centered at (x_0, y_0) at $t = 0$. The envelope in the y direction is Gaussian, whereas it is very flat with sharp edges in the x direction. The oscillating factor enables us to specify the energy of the wavepacket. The magnetic field components, compatible with the E_z field, can be found by expansion of E_z in eigenmodes of the cavity:

$$E_z(x,y,t) = \sum_{nm} \sin(k_n x)\sin(k_m y)[a_{nm}\sin(\omega t) + b_{nm}\cos(\omega t)], \tag{A.29a}$$

$$H_x(x,y,t) = \sum_{nm} \frac{ck_m}{\omega}\sin(k_n x)\cos(k_m y)[a_{nm}\cos(\omega t) - b_{nm}\sin(\omega t)], \tag{A.29b}$$

$$H_y(x,y,t) = -\sum_{nm} \frac{ck_n}{\omega}\cos(k_n x)\sin(k_m y)[a_{nm}\cos(\omega t) - b_{nm}\sin(\omega t)], \tag{A.29c}$$

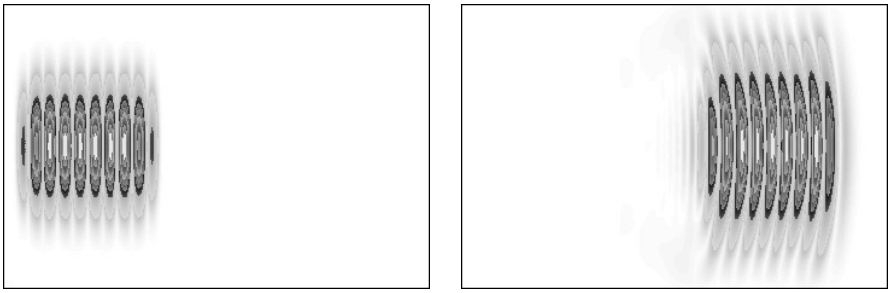

Figure A-2: Example of a wavepacket in two dimensions. The system measures $L = 18\times12$, with a mesh spacing $\delta = 0.1$. Left: energy distribution density of the initial wavepacket, with widths $\sigma = (2.75, 2.0)^T$, centered at $\mathbf{r}_0 = (3.5, 6.0)^T$ and wave-number $k = 5$. Right: energy distribution at $t = 10$, after integration with the Chebyshev algorithm ($\kappa = 10^{-13}$).

with $\omega = \omega_{nm} = c\sqrt{k_n^2 + k_m^2}$, $k_n = n\pi/L_x$ and $k_m = m\pi/L_y$. The coefficients result from evaluation of integrals, similar to 1D case,

$$a_{nm} = \frac{4}{\omega L_x L_y}\int_0^{L_x} dx \int_0^{L_y} dy \sin(k_n x)\sin(k_m y)\frac{\partial}{\partial t} f(x,y,t)|_{t=0}, \tag{A.30a}$$

$$b_{nm} = \frac{4}{L_x L_y}\int_0^{L_x} dx \int_0^{L_y} dy \sin(k_n x)\sin(k_m y) f(x,y,t=0). \tag{A.30b}$$

When we have $f(x,y,t=0) = f_1(x)f_2(y)$, the integrals in equation A.30 simplify, but not necessarily to the extent that they can be solved analytically. And even if this were the case, the summation over all the eigenmodes is still necessary, as the coefficients a_{nm} and b_{nm} couple all the modes, indicating that this procedure is numerically expensive.

As an example of a wavepacket constructed according to this procedure, and by choosing the E_z component of the TM-mode to equate the function in Eq. (A.28), see figure A-2. The divergence of the wavepacket, although mild, is clearly visible.

A.2.3 Three Dimensions

In three dimensions, in contrast with 2D, there exist localized solutions to the 3D wave-equation. For example, for a wavepacket propagating in the x-direction, of the form $f(x,y,z,t) = f_1(x-ct)f_2(y)f_3(z)$, the wave-equation reduces to

$$\frac{1}{f_2(y)}\frac{\partial^2}{\partial y^2} f_2(y) = -\frac{1}{f_3(z)}\frac{\partial^2}{\partial z^2} f_3(z), \tag{A.31}$$

for which non-zero solutions exist. However, we do not proceed with solving this equation, because it is not trivial, and it would only give us one of the fields. It is more convenient to simply extend the method of the previous section, and prepare a wavepacket by expanding a reference function in eigenmodes of the TDME of a cavity.

In three dimensions, the eigenmodes of a cavity with size L_x, L_y, L_z are

$$H_x(\mathbf{r},t) = \sum_{nml} c_{1,nml} \sin(k_n x)\cos(k_m y)\cos(k_l z) h_{nml}(t), \tag{A.32a}$$

$$H_y(\mathbf{r},t) = \sum_{nml} c_{2,nml} \cos(k_n x)\sin(k_m y)\cos(k_l z) h_{nml}(t), \tag{A.32b}$$

$$H_z(\mathbf{r},t) = \sum_{nml} c_{3,nml} \cos(k_n x)\cos(k_m y)\sin(k_l z) h_{nml}(t), \tag{A.32c}$$

$$E_x(\mathbf{r},t) = \sum_{nml} d_{1,nml} \cos(k_n x)\sin(k_m y)\sin(k_l z) e_{nml}(t), \tag{A.32d}$$

$$E_y(\mathbf{r},t) = \sum_{nml} d_{2,nml} \sin(k_n x)\cos(k_m y)\sin(k_l z) e_{nml}(t), \tag{A.32e}$$

$$E_z(\mathbf{r},t) = \sum_{nml} d_{3,nml} \sin(k_n x)\sin(k_m y)\cos(k_l z) e_{nml}(t), \tag{A.32f}$$

where

$$h_{nml}(t) = a_{nml}\cos(\omega t) - b_{nml}\sin(\omega t), \tag{A.33a}$$

$$e_{nml}(t) = a_{nml}\sin(\omega t) + b_{nml}\sin(\omega t), \tag{A.33b}$$

and $k_n = n\pi/L_x$, $k_m = m\pi/L_y$, $k_l = l\pi/L_z$ and $\omega = \omega_{nml} = c\sqrt{k_n^2 + k_m^2 + k_l^2}$. The TDME relate the sets of coefficients c_i and d_i. Omitting the *nml* indices, they yield

$$d_1\omega = k_l c_2 - k_m c_3, \tag{A.34a}$$

$$d_2\omega = k_n c_3 - k_l c_1, \tag{A.34b}$$

$$d_3\omega = k_m c_1 - k_n c_2, \tag{A.34c}$$

$$c_1\omega = k_m d_3 - k_l d_2, \tag{A.34d}$$

$$c_2\omega = k_l d_1 - k_n d_3, \tag{A.34e}$$

$$c_3\omega = k_n d_2 - k_m d_1, \tag{A.34f}$$

$$c_1 k_n + c_2 k_m + c_3 k_l = 0. \tag{A.34g}$$

One solution to this set of equations is $c_1 = k_m k_l$, $c_2 = k_n k_l$, $c_3 = -2k_n k_m$, $d_1 = k_n(2k_m^2 + k_l^2)/\omega$, $d_2 = k_m(-k_l^2 - 2k_n^2)/\omega$ and $d_3 = k_l(k_m^2 - k_n^2)/\omega$. Now we choose a reference function to fix one of the fields, for example

$$H_x(x,y,z,t) = \sin(k(x - x_0 - ct))\exp[-((x - x_0 - ct)/\sigma_x)^{10} - ((y - y_0)/\sigma_y)^2 - ((z - z_0)/\sigma_z)^2]. \tag{A.35}$$

The coefficients a_{nml} and b_{nml} can be found by integration, and the other fields are reconstructed by carrying out the summations. When the reference function decomposes, for example $f_1(x - ct) f_2(y) f_3(z)$, and we choose H_x to equate this function, we would have to evaluate the integrals

$$a_{nml} = \frac{8}{c_1 L_x L_y L_z} \int_0^{L_x} dx \sin(k_n x) f_1(x, t = 0) \int_0^{L_y} dy \cos(k_m y) f_2(y) \int_0^{L_z} dz \cos(k_l z) f_3(z), \tag{A.36a}$$

$$b_{nml} = \frac{-8}{c_1 \omega L_x L_y L_z} \int_0^{L_x} dx \sin(k_n x) \frac{\partial}{\partial t} f_1(x)|_{t=0} \int_0^{L_y} dy \cos(k_m y) f_2(y) \int_0^{L_z} dz \cos(k_l z) f_3(z). \tag{A.36b}$$

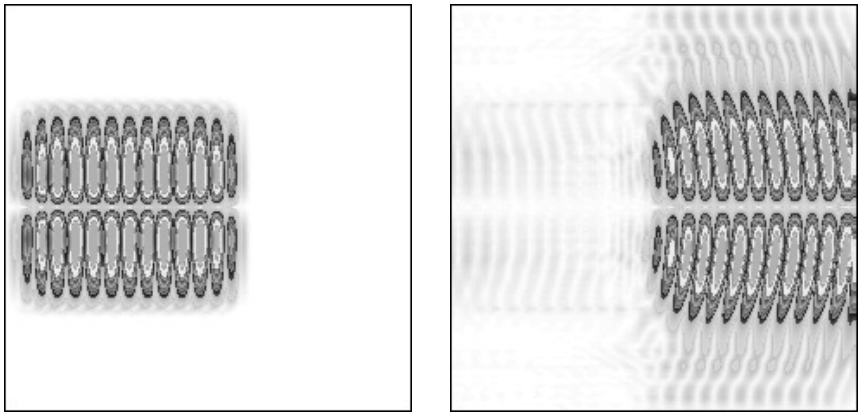

Figure A-3: Example of a wavepacket in three dimensions. System size is $L = 12 \times 12 \times 12$, with a mesh spacing $\delta = 0.1$. Left: energy distribution density slice at $y = 6$ of the initial wavepacket, with widths $\sigma = (3, 0.75, 0.75)^T$, centered at $\mathbf{r}_0 = (3.5, 6, 6)^T$ and wave-number $k = 6$. Right: energy distribution at $t = 6.4$, after integration with the Chebyshev algorithm ($\kappa = 10^{-13}$).

The integrals in the non-propagating directions can be evaluated analytically by choosing $f_2(y)$ and $f_3(z)$ appropriately. The expressions for the summations in Eq. (A.32) do not simplify however, due to the presence of the $c_i(nml)$ and $d_i(nml)$ coefficients, that couple all the modes.

A wavepacket, constructed by starting from Eq. (A.35) and reconstructing the other fields from the eigenmodes, is shown in figure A-3. As in the 2D case, the divergence of the wavepacket is clearly visible.