Gaussian packets in smooth isotropic media

Luděk Klimeš
Department of Geophysics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Praha 2, Czech Republic, E-mail: klimes@seis.karlov.mff.cuni.cz

Summary

Gaussian packets are high–frequency asymptotic space–time solutions of the wave equation. We briefly review the derivation of the evolution equations for paraxial Gaussian packets propagating in a smooth stationary non–dissipative isotropic medium. The central point of a Gaussian packet moves along the spatial central ray according to the ray tracing equations. The first derivatives of the complex–valued phase function of the Gaussian packet at the central point are determined by ray tracing, and are real–valued. The shape of a Gaussian packet is determined by the second derivatives of the complex–valued phase function. The equations for these second derivatives, derived in general Cartesian coordinates, nicely decouple in ray–centred coordinates. The 2×2 matrix of the second derivatives of the phase function in the plane perpendicular to the central ray describes the Gaussian beam corresponding to the Gaussian packet, and is calculated by dynamic ray tracing in the same way as for the Gaussian beam. The evolution of the remaining second derivatives of the phase function of the Gaussian packet may be expressed in terms of the complex–valued matrix of geometrical spreading of the Gaussian beam.

Keywords

Gaussian packets, Gaussian beams, space–time ray theory, complex–valued phase function, inhomogeneous media.

1. Introduction

Gaussian packets, also called (space–time) Gaussian beams (Ralston, 1983), quasiphotons (Babich & Ulin, 1981) or coherent states (Combescure, Ralston & Robert, 1999), are high–frequency asymptotic space–time solutions of the wave equation (e.g., elastodynamic equation, system of Maxwell equations). Their envelopes at any given time are nearly Gaussian functions. A Gaussian packet is concentrated to a real–valued space–time ray, like a Gaussian beam to a spatial ray. In a stationary medium, a Gaussian packet propagates along its real–valued spatial central ray. A Gaussian packet has an approximately Gaussian profile in all spatial directions and in time. A paraxial Gaussian packet is a Gaussian packet approximated by the paraxial ray approximation in the vicinity of its central point.

The equations for the evolution of a Gaussian packet were derived by Babich & Ulin (1981) and Ralston (1983). Here we briefly review the derivation of the equations for paraxial Gaussian packets propagating in smooth stationary non–dissipative isotropic media.

The evolution equations are required to propagate Gaussian packets constituting a general time–domain wavefield (Žáček, 2003), and to optimize the shape of Gaussian

In: Seismic Waves in Complex 3-D Structures, Report 14 (Department of Geophysics, Charles University, Prague, 2004), pp. 43–54

packets (Žáček, 2001). The evolution equations are unnecessary for the asymptotic decomposition of the time–harmonic wavefield specified in terms of amplitude and phase (Klimeš, 1984, 1989), but may be applied to the optimization of the shape of Gaussian packets used in this asymptotic decomposition.

The central point of a Gaussian packet moves along the spatial central ray according to the ray tracing equations. The phase function and its first derivatives at the central point of the Gaussian packet are determined by ray tracing and are real–valued in non–dissipative media. The shape of a Gaussian packet is determined by the second derivatives of the phase function. Evolution of the complex–valued second derivatives of the phase function, which control the shape of the Gaussian packet, along the central ray is determined by quantities calculated by dynamic ray tracing. Infinitely long paraxial Gaussian packets correspond to the paraxial approximations of Gaussian beams. Infinitely broad paraxial Gaussian packets correspond to the paraxial approximations of space–time ray–theory wavefields.

2. Gaussian packet and the space-time eikonal equation

A Gaussian packet is an approximate space–time high–frequency asymptotic solution of the corresponding hyperbolic wave equation, and may be expressed in the form of

$$\mathbf{U} = \mathbf{A} \exp(\mathrm{i}\omega\tau) \quad , \tag{1}$$

where both complex–valued vectorial amplitude $\mathbf{A} = \mathbf{A}(x_\alpha)$ and complex–valued phase function $\tau = \tau(x_\alpha)$ are smooth functions of the four space–time coordinates x_α. Hereinafter, the lower–case Greek subscripts ${}_{\alpha,\beta,\ldots} = {}_{1,2,3,4}$ will correspond to four space–time coordinates: spatial coordinates x_i with ${}_i = {}_{1,2,3}$, and time x_4.

The complex–valued phase function satisfies the space–time eikonal equation

$$v^2 \tau_{,i}\tau_{,i} - \tau_{,4}\tau_{,4} = 0 \quad . \tag{2}$$

Introducing space–time slowness vector

$$N_\alpha = \tau_{,\alpha} \tag{3}$$

and Hamiltonian $H = H(x_\alpha, N_\alpha)$, the eikonal equation may be solved by the method of characteristics. The corresponding Hamilton space–time ray tracing equations for temporally independent propagation velocity $v = v(x_k)$ are

$$\frac{\mathrm{d}y_i}{\mathrm{d}t} = [v(y_k)]^2 N_i \ , \quad \frac{\mathrm{d}y_4}{\mathrm{d}t} = -N_4 \ , \quad \frac{\mathrm{d}N_i}{\mathrm{d}t} = -[v(y_n)]^{-1} v_{,i}(y_k) \ , \quad \frac{\mathrm{d}N_4}{\mathrm{d}t} = 0 \ . \tag{4}$$

Here we have denoted the space–time coordinates by y_α instead of x_α in order to be able to distinguish the points of the space–time ray from general space–time coordinates x_α.

The imaginary part of the phase function τ must have, at a fixed time $x_4 = y_4(t)$, a strict minimum over space at some point $x_i = y_i(t)$. The imaginary part of the phase function can be approximated in the vicinity of its minimum y_i by the quadratic form of spatial distances $[x_i - y_i(t)]$. For sufficiently high frequencies, the amplitude profile of the Gaussian packet is thus *nearly* Gaussian in space and concentrated close to the point $y_i(t)$. We shall call the point $y_i(t)$ the central point of the Gaussian packet.

Since the Hamiltonian is constant along the space–time rays, the complex–valued phase function is constant, too. In this way, the minimum of the imaginary part of τ, which gives the maximum of the high–frequency Gaussian packet, is identical with the space–time ray passing through the point $y_i(t^0)$ at time $y_4(t^0)$ (Norris, White & Schreiffer, 1987). We shall assume that the value of the phase function at this space–time ray is zero,

$$\tau[y_i(t)] = 0 \quad . \tag{5}$$

Since (5) corresponds to the minimum of the imaginary part of τ, inequality

$$\mathrm{Im}[\tau(x_i)] \geq 0 \tag{6}$$

is a consequence of option (5).

The Gaussian packet is thus concentrated close to the space–time ray as the Gaussian beam is concentrated close to the spatial ray, and is also called a (space–time) Gaussian beam (Ralston 1983). Thus, in a time–independent model, a Gaussian packet is moving along the spatial ray with the ray velocity. The Gaussian packet remains approximately Gaussian in space at all times $x_4 = y_4(t)$. At any time, the principal part of the energy of the Gaussian packet is effectively concentrated in some vicinity of the central point $y_i(t)$ of the Gaussian packet. This vicinity is called the *effective region* of the Gaussian packet. At a specified time, the effective region of a Gaussian packet is limited in space and, for a sufficiently high frequency, it is concentrated close to its central point. In space–time, however, the effective region of a Gaussian packet is not limited.

We select

$$N_4 = -1 \quad . \tag{7}$$

Derivative $\frac{\mathrm{d}}{\mathrm{d}t}$ along the space–time ray then coincides with derivative $\frac{\mathrm{d}}{\mathrm{d}y_4}$ with respect to time y_4, and space–time ray tracing equations (4) reduce to the spatial ray tracing equations.

3. Paraxial Gaussian packet

We shall refer to the approximation of a Gaussian packet, obtained by substituting the exact phase function τ by its Taylor expansion, as the paraxial approximation of the Gaussian packet or, briefly, as the *paraxial Gaussian packet*. The paraxial approximation of the Gaussian packet in space is an analogy to the paraxial approximation of the Gaussian beam in the plane perpendicular to the ray. We shall refer to the Gaussian packet (1) with the exact phase function τ satisfying the eikonal equation (2) as the *strict Gaussian packet*.

The space–time paraxial approximation of a Gaussian packet centred at point $y_\alpha(t)$, is

$$\mathbf{U} = \mathbf{A} \, \exp\{\mathrm{i}\omega[N_\alpha r_\alpha + \tfrac{1}{2} N_{\alpha\beta} r_\alpha r_\beta]\} \quad , \tag{8}$$

where

$$r_i = x_i - y_i(t) \quad , \tag{9}$$

$$r_4 = x_4 - y_4(t) = x_4 - t \quad , \tag{10}$$

$$N_{\alpha\beta} = \tau_{,\alpha\beta} \quad , \tag{11}$$

and N_α defined by (3) is the space–time slowness vector of the Gaussian packet. Quantities $\mathbf{A}$, N_α and $N_{\alpha\beta}$ on the right–hand side of equation (8) are taken at the central point $y_\alpha(t)$ of a Gaussian packet.

The spatial effective region of the Gaussian packet may be sufficiently small for sufficiently high frequencies. Then, at any time $x_4 = y_4(t)$, the phase function τ of the (strict) Gaussian packet can be replaced, in the spatial effective region, by its Taylor expansion up to the second order with respect to the spatial coordinates,

$$\mathbf{U} = \mathbf{A}\ \exp\{\mathrm{i}\omega[N_i r_i + \tfrac{1}{2}N_{ij}r_i r_j]\} \quad , \tag{12}$$

where N_{ij} is the spatial part of the 4×4 matrix (11) of the second space–time derivatives of the phase function.

The difference between the strict Gaussian packet and its spatial paraxial approximation is of the asymptotic order $\omega^{-\frac{1}{2}}$. A single paraxial Gaussian packet is then a worse solution to the equations of motion than the strict Gaussian packet by the asymptotic order $\omega^{\frac{1}{2}}$. However, the differences of the order $\omega^{-\frac{1}{2}}$ between the paraxial and strict Gaussian packets are odd functions of the coordinates and so vanish in the integration over the space in the asymptotic decomposition into Gaussian packets. The error of the 3–parametric (2–parametric in 2-D models) time–harmonic superposition of paraxial Gaussian packets is thus of the asymptotic order ω^{-1}, i.e. of the same order as the error of the superposition of the strict Gaussian packets.

Like the phase function, the amplitude can also be replaced by its Taylor expansion. The restriction of the amplitude up to the n^{th} order introduces an error of the asymptotic order $\omega^{-\frac{n+1}{2}}$. Since the error of the second order expansion of the phase function is of the order $\omega^{-\frac{1}{2}}$, the amplitude can be replaced by the constant in the paraxial approximation.

4. Equations for the second derivatives of phase function in Cartesian coordinates

The Ricatti equation for the 4×4 space–time matrix (11) may be obtained by differentiating twice the eikonal equation (2) with respect to the space–time coordinates x_α, see Ralston (1983, eq. 2.4). The corresponding linear dynamic ray tracing system may be obtained by differentiating the ray tracing system with respect to the space–time ray parameters, see Ralston (1983, eq. 2.6). The Ricatti equation for the 4×4 space–time matrix (11) may be reduced to the Ricatti equation for its 3×3 spatial submatrix N_{ij}, see Kachalov (1984, eq. 9), Babich, Buldyrev & Molotkov (1985, eq. 2.15), Norris, White & Schreiffer (1987, eq. 2.27a). For the corresponding linear dynamic ray tracing system refer to Kachalov (1984, eq. 12), Babich, Buldyrev & Molotkov (1985, eq. 2.18), Norris, White & Schreiffer (1987, eq. 2.25ab). Here we shall directly derive the Ricatti equation for the 3×3 spatial submatrix of matrix (11) and then switch to ray–centred coordinates in order to decouple it.

Differentiating eikonal equation (2) with respect to space–time coordinates, we arrive at

$$vv_{,\alpha}\tau_{,i}\tau_{,i} + v^2\tau_{,i\alpha}\tau_{,i} - \tau_{,4\alpha}\tau_{,4} = 0 \quad . \tag{13}$$

Since we selected $\tau_{,4} = -1$, see (7), equation (13) yields relation

$$\tau_{,4\alpha} = -v^{-1}v_{,\alpha} - v^2\tau_{,i}\tau_{,i\alpha} \quad . \tag{14}$$

Differentiating twice eikonal equation (2) with respect to spatial coordinates, we arrive at equation

$$[vv_{,jk}+v_{,j}v_{,k}]\tau_{,i}\tau_{,i}+2vv_{,j}\tau_{,ik}\tau_{,i}+2vv_{,k}\tau_{,ij}\tau_{,i}+v^2[\tau_{,ijk}\tau_{,i}+\tau_{,ij}\tau_{,ik}]-\tau_{,4jk}\tau_{,4}-\tau_{,4j}\tau_{,4k} = 0 \ . \tag{15}$$

Insertion of space–time ray tracing equations (4) into equation $\mathrm{d}\tau_{,jk}/\mathrm{d}t = \tau_{,ij\alpha}\mathrm{d}y_\alpha/\mathrm{d}t$ yields

$$\frac{\mathrm{d}\tau_{,jk}}{\mathrm{d}t} = v^2\tau_{,ijk}\tau_{,i} - \tau_{,4jk}\tau_{,4} \quad . \tag{16}$$

Inserting (15) with (14) into (16), we arrive at

$$\begin{aligned}\frac{\mathrm{d}\tau_{,jk}}{\mathrm{d}t} = &- v^2\tau_{,ij}\tau_{,ik} - v^{-2}[vv_{,jk} + v_{,j}v_{,k}] - 2vv_{,j}\tau_{,ik}\tau_{,i} - 2vv_{,k}\tau_{,ij}\tau_{,i} \\ &+ v^{-2}v_{,j}v_{,k} + vv_{,j}\tau_{,ik}\tau_{,i} + vv_{,k}\tau_{,ij}\tau_{,i} + v^4\tau_{,i}\tau_{,ij}\tau_{,lk}\tau_{,l} \quad ,\end{aligned} \tag{17}$$

which can be rearranged to obtain the Ricatti equation

$$\frac{\mathrm{d}\tau_{,jk}}{\mathrm{d}t} = -v^2\tau_{,ij}\tau_{,ik} - v^{-1}v_{,jk} - vv_{,j}\tau_{,ik}\tau_{,i} - vv_{,k}\tau_{,ij}\tau_{,i} + v^4\tau_{,i}\tau_{,ij}\tau_{,lk}\tau_{,l} \quad . \tag{18}$$

In notation (3) and (11), Ricatti equation (18) reads

$$\frac{\mathrm{d}N_{jk}}{\mathrm{d}t} = -v^2N_{ij}N_{ik} - v^{-1}v_{,jk} - vv_{,j}N_{ik}N_i - vv_{,k}N_{ij}N_i + v^4N_iN_{ij}N_{lk}N_l \quad , \tag{19}$$

and relation (14) yields relations

$$N_{i4} = N_{4i} = -v^2N_{ij}N_j - v^{-1}v_{,i} \tag{20}$$

and

$$N_{44} = -v^2N_{4j}N_j = v^4N_iN_{ij}N_j + vN_iv_{,i} \quad . \tag{21}$$

Equations (19), (20) and (21) describe the evolution of the shape of a Gaussian packet in general Cartesian coordinates.

5. Equations for the second derivatives of phase function in ray–centred coordinates

We denote by h_{im} the i^{th} component of m^{th} basis vector of the ray centred coordinate system. The basis vectors are orthonormal. Basis vectors h_{i1} and h_{i2} are perpendicular to the central ray and are calculated by numerical integration (Červený, Klimeš & Pšenčík, 1988, eq. 5.6; Červený, 2001, eq. 4.1.5). Basis vector $h_{i3} = N_i/\sqrt{N_kN_k}$ is tangent to the central ray.

Covariant derivatives M_{mn} of the phase function in ray–centred coordinates are related to the partial derivatives N_{mn} in Cartesian coordinates through equations

$$M_{mn} = N_{jk}h_{jm}h_{kn} \quad , \tag{22}$$

$$N_{jk} = h_{jm}h_{kn}M_{mn} \quad , \tag{23}$$

$$M_{m4} = N_{j4}h_{jm} \quad , \tag{24}$$

$$N_{j4} = h_{jm}M_{m4} \quad , \tag{25}$$

$$M_{44} = N_{44} \quad . \tag{26}$$

Ricatti equation (19) for matrix N_{ij} is equivalent to the Ricatti equation for 3×3 matrix M_{mn}, see Norris, White & Schreiffer (1987, eq. 4.8d), with the corresponding linear dynamic ray tracing system (Norris, White & Schreiffer, 1987, eq. 4.8ab). Analogous Ricatti equation for the 3×3 matrix of the second partial derivatives in ray–centred coordinates was derived by Babich & Ulin (1981, eqs. 2.7–2.9). The evolution equations for the 2×2 submatrix M_{MN}, corresponding to the plane perpendicular to the ray, are decoupled, i.e. they do not depend upon the outer elements M_{m3}. These equations are identical with the equations for Gaussian beams and can be treated in the same way. The equations for M_{m3} can be solved analytically (Babich and Ulin, 1981). Here we shall stick to the equations for the 3×3 matrix of the second covariant derivatives (22) in ray–centred coordinates.

Equations (20) and (21) read

$$M_{i4} = -vM_{i3} - v^{-1}V_i \tag{27}$$

and

$$M_{44} = v^2 M_{33} + V_3 \quad , \tag{28}$$

where

$$V_m = v_{,i} h_{im} \tag{29}$$

is the velocity gradient in ray–centred coordinates. The derivatives of the basis vectors of the ray–centred coordinate system along the ray satisfy relations

$$\frac{\mathrm{d}h_{jM}}{\mathrm{d}t} h_{jN} = 0 \ , \quad \frac{\mathrm{d}h_{j3}}{\mathrm{d}t} h_{jN} = -V_N \ , \quad \frac{\mathrm{d}h_{jM}}{\mathrm{d}t} h_{j3} = V_M \ , \quad \frac{\mathrm{d}h_{j3}}{\mathrm{d}t} h_{j3} = 0 \ . \tag{30}$$

Equation (18), transformed using (22) and (23) into ray–centred coordinates, reads

$$\frac{\mathrm{d}M_{mn}}{\mathrm{d}t} = -M_{jn}\frac{\mathrm{d}h_{ij}}{\mathrm{d}t} h_{im} - M_{mk}\frac{\mathrm{d}h_{ik}}{\mathrm{d}t} h_{in} - v^2 M_{Km} M_{Kn} - v^{-1} V_{mn} - V_m M_{3n} - V_n M_{3m} \ , \tag{31}$$

where

$$V_{mn} = v_{,ij} h_{im} h_{jn} \tag{32}$$

are the covariant velocity derivatives in ray–centred coordinates. Inserting (30) for the derivatives of the basis vectors, equation (32) may be expanded into three equations

$$\frac{\mathrm{d}M_{MN}}{\mathrm{d}t} = M_{3N}V_M + M_{M3}V_N - v^2 M_{MK}M_{KN} - v^{-1}V_{MN} - V_M M_{N3} - V_N M_{M3} \ , \tag{33}$$

$$\frac{\mathrm{d}M_{M3}}{\mathrm{d}t} = M_{33}V_M - M_{MK}V_K - v^2 M_{MI}M_{I3} - v^{-1}V_{M3} - V_M M_{33} - V_3 M_{M3} \ , \tag{34}$$

$$\frac{\mathrm{d}M_{33}}{\mathrm{d}t} = -2M_{I3}V_I - v^2 M_{3I}M_{I3} - v^{-1}V_{33} - 2V_3 M_{33} \quad . \tag{35}$$

Equations (33) to (35) may be expressed in the form

$$\frac{\mathrm{d}M_{MN}}{\mathrm{d}t} = -v^2 M_{MK}M_{KN} - v^{-1}V_{MN} \quad , \tag{36}$$

$$\frac{\mathrm{d}M_{M3}}{\mathrm{d}t} = -M_{Mi}V_i - v^2 M_{MI}M_{I3} - v^{-1}V_{M3} \quad , \tag{37}$$

$$\frac{\mathrm{d}M_{33}}{\mathrm{d}t} = -2M_{i3}V_i - v^2 M_{3I}M_{I3} - v^{-1}V_{33} \quad . \tag{38}$$

The covariant velocity derivatives V_i and V_{ij} in ray–centred coordinates are defined by equations (29) and (32). Equations (36) to (38) for the second covariant derivatives in ray–centred coordinates are equivalent to the equations by Babich & Ulin (1981, eqs. 2.7–2.9) for the second partial derivatives in ray–centred coordinates.

Equation (36) is identical with the Ricatti equation for a Gaussian beam. Equations (37) and (38) extend the Gaussian–beam solution to a Gaussian–packet solution.

6. Solving the equation for a Gaussian beam

To express equations (36) to (38) in the vector and matrix notation, we introduce following matrices and vectors

$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \quad , \tag{39}$$

$$\mathbf{M}_3 = \begin{pmatrix} M_{13} \\ M_{23} \end{pmatrix} \quad , \tag{40}$$

$$\mathbf{W} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \quad , \tag{41}$$

$$\mathbf{V} = \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \quad . \tag{42}$$

Equation (36) in the matrix notation reads

$$\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t} = -v^2\mathbf{M}\mathbf{M} - v^{-1}\mathbf{W} \quad , \tag{43}$$

and is *identical with the corresponding equation for Gaussian beams.* Its solution may be expressed in form

$$\mathbf{M} = \mathbf{M}^{\mathrm{T}} = \mathbf{P}\mathbf{Q}^{-1} \quad , \tag{44}$$

where matrices $\mathbf{Q}$ and $\mathbf{P}$ satisfy the dynamic ray tracing equations

$$\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}t} = v^2\mathbf{P} \quad , \qquad \frac{\mathrm{d}\mathbf{P}}{\mathrm{d}t} = -v^{-1}\mathbf{W}\mathbf{Q} \quad . \tag{45}$$

Introducing the paraxial–ray propagator matrix

$$\begin{pmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{P}_1 & \mathbf{P}_2 \end{pmatrix} \quad , \tag{46}$$

which is the solution of dynamic ray tracing equations (45) with unit initial conditions

$$\begin{pmatrix} \mathbf{Q}_1^0 & \mathbf{Q}_2^0 \\ \mathbf{P}_1^0 & \mathbf{P}_2^0 \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \quad , \tag{47}$$

matrices $\mathbf{Q}$ and $\mathbf{P}$ may be expressed in terms of their initial values $\mathbf{Q}^0$ and $\mathbf{P}^0$ as

$$\mathbf{Q} = \mathbf{Q}_1\,\mathbf{Q}^0 + \mathbf{Q}_2\,\mathbf{P}^0 \quad , \qquad \mathbf{P} = \mathbf{P}_1\,\mathbf{Q}^0 + \mathbf{P}_2\,\mathbf{P}^0 \quad , \tag{48}$$

with

$$\mathbf{P}^0 = \mathbf{M}^0\,\mathbf{Q}^0 \quad . \tag{49}$$

Matrix (44) may then be expressed in the form

$$\mathbf{M} = (\mathbf{P}_1 + \mathbf{P}_2\,\mathbf{M}^0)\,(\mathbf{Q}_1 + \mathbf{Q}_2\,\mathbf{M}^0)^{-1} \quad . \tag{50}$$

7. Solving the equations for a Gaussian packet

To solve equations (37) and (38), we calculate the expressions for the derivatives of V_i along the central ray,

$$\frac{\mathrm{d}V_M}{\mathrm{d}t} = \frac{\mathrm{d}[v_{,j}\, h_{jM}]}{\mathrm{d}t} = v v_{,jk} h_{jM} h_{k3} + v_{,j} \frac{\mathrm{d}h_{jM}}{\mathrm{d}t} = v V_{M3} + V_M V_3 \quad , \tag{51}$$

$$\frac{\mathrm{d}[v^{-1} V_M]}{\mathrm{d}t} = V_{M3} \quad , \tag{52}$$

$$\frac{\mathrm{d}V_3}{\mathrm{d}t} = \frac{\mathrm{d}[v_{,j}\, h_{j3}]}{\mathrm{d}t} = v v_{,jk} h_{j3} h_{k3} + v_{,j} \frac{\mathrm{d}h_{j3}}{\mathrm{d}t} = v V_{33} - V_K V_K \quad . \tag{53}$$

Using (52), equation (37) may be rewritten in the vector and matrix notation in the form

$$\frac{\mathrm{d}\mathbf{M}_3}{\mathrm{d}t} = -V_3 \mathbf{M}_3 - v^2 \mathbf{M}[\mathbf{M}_3 + v^{-2}\mathbf{V}] - v^{-1} \frac{[\mathrm{d}v^{-1}\mathbf{V}]}{\mathrm{d}t} \quad , \tag{54}$$

which may further be converted into

$$\frac{\mathrm{d}[v\,\mathbf{M}_3]}{\mathrm{d}t} = -v^2 \mathbf{M}[v\mathbf{M}_3 + v^{-1}\mathbf{V}] - \frac{[\mathrm{d}v^{-1}\mathbf{V}]}{\mathrm{d}t} \quad , \tag{55}$$

and subsequently into

$$\frac{\mathrm{d}[v\mathbf{M}_3 + v^{-1}\mathbf{V}]}{\mathrm{d}t} = -v^2 \mathbf{M}[v\mathbf{M}_3 + v^{-1}\mathbf{V}] \quad . \tag{56}$$

Considering relation

$$\frac{\mathrm{d}(\mathbf{Q}^{\mathrm{T}})^{-1}}{\mathrm{d}t} = -v^2 (\mathbf{Q}^{\mathrm{T}})^{-1} \mathbf{P}^{\mathrm{T}} (\mathbf{Q}^{\mathrm{T}})^{-1} = -v^2 \mathbf{M} (\mathbf{Q}^{\mathrm{T}})^{-1} \quad , \tag{57}$$

following from (44) and (45), we see that the solution of equation (57) is

$$\mathbf{M}_3 = v^{-1} \left[(\mathbf{Q}^{\mathrm{T}})^{-1} \mathbf{C} - v^{-1} \mathbf{V} \right] \quad , \tag{58}$$

where $\mathbf{C}$ is a constant vector determined by the initial conditions. Equation (38) in the vector and matrix notation reads

$$\frac{\mathrm{d}M_{33}}{\mathrm{d}t} = -2V_3 M_{33} - v^2 [\mathbf{M}_3 + v^{-2}\mathbf{V}]^{\mathrm{T}} [\mathbf{M}_3 + v^{-2}\mathbf{V}] + v^{-2} \mathbf{V}^{\mathrm{T}} \mathbf{V} - v^{-1} V_{33} \quad . \tag{59}$$

Using (53) and inserting (58), equation (59) takes the form of

$$\frac{\mathrm{d}M_{33}}{\mathrm{d}t} = -2V_3 M_{33} - \mathbf{C}^{\mathrm{T}} \mathbf{Q}^{-1} (\mathbf{Q}^{\mathrm{T}})^{-1} \mathbf{C} - v^{-2} \frac{\mathrm{d}V_3}{\mathrm{d}t} \quad , \tag{60}$$

which may further be converted into

$$\frac{\mathrm{d}(v^2 M_{33} + V_3)}{\mathrm{d}t} = -v^2 \mathbf{C}^{\mathrm{T}} \mathbf{Q}^{-1} (\mathbf{Q}^{\mathrm{T}})^{-1} \mathbf{C} \quad . \tag{61}$$

Considering relation

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{\mathrm{i}}{2} \mathbf{Q}^{-1} (\mathrm{Im}\mathbf{M})^{-1} (\mathbf{Q}^{\mathrm{T}})^{-1} \right] = v^2\; \mathbf{Q}^{-1} (\mathbf{Q}^{\mathrm{T}})^{-1} \quad , \tag{62}$$

following from (43) and (57), we see that

$$M_{33} = v^{-2} \left[-\frac{\mathrm{i}}{2} \mathbf{C}^{\mathrm{T}} \mathbf{Q}^{-1} (\mathrm{Im}\mathbf{M})^{-1} (\mathbf{Q}^{\mathrm{T}})^{-1} \mathbf{C} + C - V_3 \right] \quad , \tag{63}$$

where C is the integration constant. Denoting

$$\mathbf{M}_4 = \begin{pmatrix} M_{14} \\ M_{24} \end{pmatrix} \quad , \tag{64}$$

and combining equations (58) and (63) with equations (27) and (28), we may write equations for elements $\mathbf{M}_3$, $\mathbf{M}_4$, M_{33}, M_{34} and M_{44}, supplementing 2×2 Gaussian–beam matrix (44) to the 4×4 Gaussian–packet matrix $M_{\alpha\beta}$, in the form of two explicit evolution equations

$$\mathbf{M}_4 = -(\mathbf{Q}^{\mathrm{T}})^{-1}\mathbf{C} \tag{65}$$

(Babich & Ulin, 1981, eq. 2.13),

$$M_{44} = -\frac{\mathrm{i}}{2}\mathbf{C}^{\mathrm{T}}\mathbf{Q}^{-1}(\mathrm{Im}\mathbf{M})^{-1}(\mathbf{Q}^{\mathrm{T}})^{-1}\mathbf{C} + C \quad , \tag{66}$$

and three simple relations

$$\mathbf{M}_3 = -v^{-1}\mathbf{M}_4 - v^{-2}\mathbf{V} \quad , \tag{67}$$

$$M_{34} = -v^{-1}M_{44} \quad , \tag{68}$$

$$M_{33} = v^{-2}[M_{44} - V_3] \quad . \tag{69}$$

The second covariant derivatives of phase function in ray–centred coordinates are given by equation (50) and equations (65) to (69). The derivatives may be transformed into general Cartesian coordinates using equations (23), (25) and (26).

Equation (66) may also be expressed in terms of vector (65),

$$M_{44} = -\frac{\mathrm{i}}{2}\mathbf{M}_4^{\mathrm{T}}\,(\mathrm{Im}\mathbf{M})^{-1}\mathbf{M}_4 + C \quad . \tag{70}$$

Constants $\mathbf{C}$ and C are determined by the initial values $\mathbf{M}_4^0$ and M_{44}^0 of elements $\mathbf{M}_4$ and M_{44} through equations (65) and (70),

$$\mathbf{C} = -{\mathbf{Q}^0}^{\mathrm{T}}\mathbf{M}_4^0 \quad , \tag{71}$$

$$C = M_{44}^0 + \frac{\mathrm{i}}{2}{\mathbf{M}_4^0}^{\mathrm{T}}(\mathrm{Im}\mathbf{M}^0)^{-1}\mathbf{M}_4^0 \quad , \tag{72}$$

where $\mathbf{Q}^0$ is the initial value of complex–valued matrix $\mathbf{Q}$.

Since

$$\mathbf{Q}(\mathbf{Q}^0)^{-1} = \mathbf{Q}_1 + \mathbf{Q}_2\mathbf{M}^0 \quad , \tag{73}$$

equation (65) with (71) may be expressed as

$$\mathbf{M}_4 = [(\mathbf{Q}_1 + \mathbf{Q}_2\mathbf{M}^0)^{-1}]^{\mathrm{T}}\mathbf{M}_4^0 \quad . \tag{74}$$

Non–vanishing vector (74) implies that the Gaussian packet is asymmetric with respect to the central ray. The evolution of the shape of a Gaussian packet along the central ray is illustrated in Figure 1.

Since matrix

$$\mathbf{Q}^{\mathrm{T}}\mathrm{Im}\mathbf{M}\;\mathbf{Q}^* = {\mathbf{Q}^0}^{\mathrm{T}}\mathrm{Im}\mathbf{M}^0\;{\mathbf{Q}^0}^* \quad , \tag{75}$$

where $\mathbf{Q}^*$ is the complex–conjugate matrix to $\mathbf{Q}$, is constant along the ray, equation (66) may also be expressed as

$$M_{44} = -\frac{\mathrm{i}}{2}\mathbf{C}^{\mathrm{T}}\mathbf{Q}^{-1}\mathbf{Q}^*({\mathbf{Q}^0}^*)^{-1}(\mathrm{Im}\mathbf{M}^0)^{-1}({\mathbf{Q}^0}^{\mathrm{T}})^{-1}\mathbf{C} + C \tag{76}$$

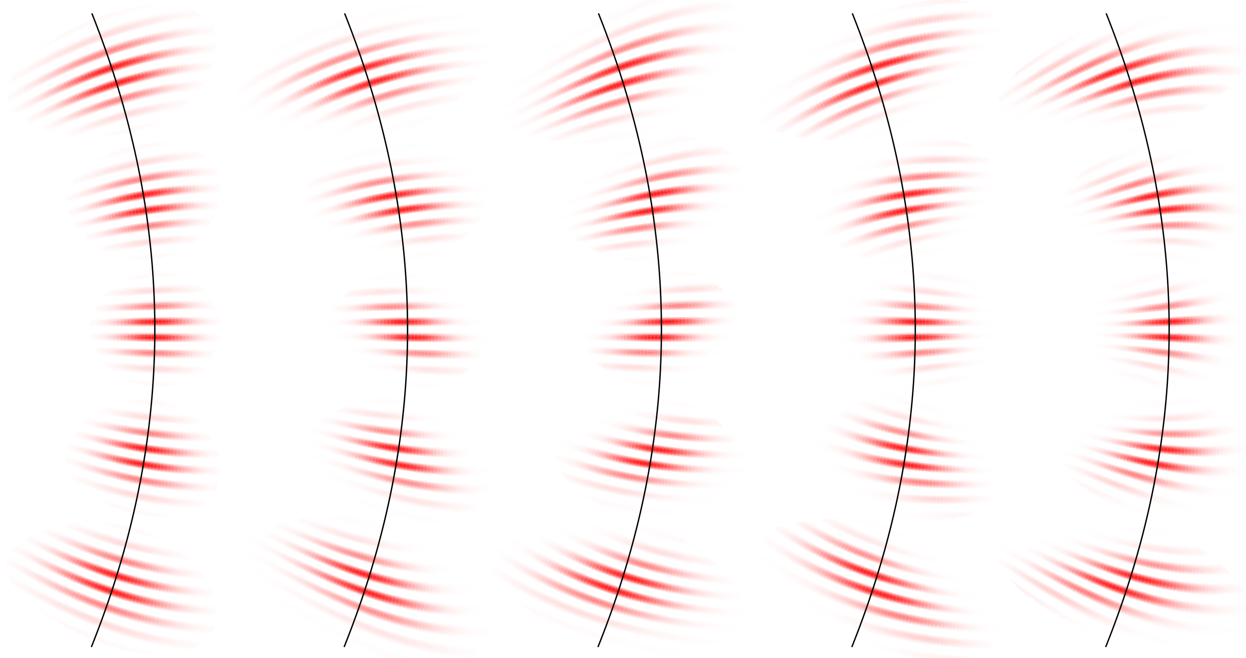

Figure 1. Symmetric and asymmetric Gaussian packets propagating along a spatial ray. All five packets correspond to Gaussian beams of equal shapes. The first Gaussian packet is axially symmetric with respect to its central ray. The second and third packets have envelopes oblique with respect to their central rays. The frequencies of the second and third packets at the waists of the corresponding Gaussian beams are symmetric with respect to the central rays. The fourth and fifth packets have different frequencies to the left and to the right from the central rays. We may call them "dispersive". The envelopes of the fourth and fifth packets at the waists of the corresponding Gaussian beams are symmetric with respect to the central rays. During the evolution of Gaussian packets, the dispersion of the wavefronts generates obliquity of the envelopes and vice versa. The asymmetric Gaussian packets are thus both oblique and dispersive in general.

(Babich & Ulin, 1981, eq. 2.13), and subsequently as

$$M_{44} = -\frac{\mathrm{i}}{2}\mathbf{M}_4^{\mathrm{T}}\left[\mathbf{Q}(\mathbf{Q}^0)^{-1}\right]^*(\mathrm{Im}\mathbf{M}^0)^{-1}\mathbf{M}_4^0 + C \quad . \tag{77}$$

Inserting (72) into (77), we obtain equation

$$M_{44} = M_{44}^0 + \frac{\mathrm{i}}{2}\mathbf{M}_4^{\mathrm{T}}\left\{\mathbf{Q}(\mathbf{Q}^0)^{-1} - \left[\mathbf{Q}(\mathbf{Q}^0)^{-1}\right]^*\right\}(\mathrm{Im}\mathbf{M}^0)^{-1}\mathbf{M}_4^0 \quad . \tag{78}$$

Inserting (73) into (78), we arrive at simple expression

$$M_{44} = M_{44}^0 - \mathbf{M}_4^{\mathrm{T}}\mathbf{Q}_2\,\mathbf{M}_4^0 \quad . \tag{79}$$

After insertion of (74), equation (79) takes the form

$$M_{44} = M_{44}^0 - {\mathbf{M}_4^0}^{\mathrm{T}}(\mathbf{Q}_1 + \mathbf{Q}_2\mathbf{M}^0)^{-1}\mathbf{Q}_2\,\mathbf{M}_4^0 \quad . \tag{80}$$

Equation (74) is convenient for calculation of vector $\mathbf{M}_4$ along the central spatial ray. To calculate M_{44}, we may use, e.g., equation (70) with (72), or equation (79), or equation (80). Quantities $\mathbf{M}_3$, M_{33} and M_{34} can then be obtained through simple relations (67) to (69).

8. Amplitude of a Gaussian packet

The vectorial amplitude $\mathbf{A}$ of the Gaussian packet may be expressed in terms of the complex–valued scalar amplitude A and unit polarization vector $\mathbf{e}$,

$$\mathbf{A} = A\,\mathbf{e} \quad . \tag{81}$$

The unit polarization vector $\mathbf{e}$ is identical to the analogous polarization vector of a Gaussian beam and to the ray–theory polarization vector.

The complex–valued scalar amplitude evolves along the central ray according to equation (Babich & Ulin, 1981)

$$A = A^0 \sqrt{\frac{v^0\,\varrho^0\,\det(\mathbf{Q}^0)}{v\,\varrho\,\det(\mathbf{Q})}} \quad . \tag{82}$$

Considering (73), we may also write equation (82) in form

$$A = A^0 \sqrt{\frac{v^0\,\varrho^0}{v\,\varrho\,\det(\mathbf{Q}_1 + \mathbf{Q}_2\mathbf{M}^0)}} \quad . \tag{83}$$

Here velocity v and density ϱ correspond to the elastodynamic equation, and should be replaced by respective material parameters for other wave equations.

Acknowledgements

The research has been supported by the Grant Agency of the Czech Republic under Contracts 205/01/D097 and 205/04/1104, by the Grant Agency of the Charles University under Contract 375/2004/B-GEO/MFF, by the Ministry of Education of the Czech Republic within Research Project MSM113200004, and by the members of the consortium "Seismic Waves in Complex 3-D Structures" (see "http://sw3d.mff.cuni.cz").

References

Babich, V.M. & Ulin, V.V. (1981): Complex space–time ray method and "quasiphotons" (in Russian). *Zap. Nauchn. Sem. Leningr. Otd. Mat. Instit.*, **117**, 5–12, english transl.: *J. Sov. Math.*, **24**(1984), 269–273.

Babich, V.M., Buldyrev, V.S. & Molotkov, I.A. (1985): *Space–time Ray Method. Linear and Non–linear Waves* (in Russian). Leningrad Univ. Press.

Červený, V. (2001): *Seismic Ray Theory.* Cambridge Univ. Press, Cambridge.

Červený, V., Klimeš, L. & Pšenčík, I. (1988): Complete seismic–ray tracing in three–dimensional structures. In: Doornbos, D.J. (ed.): *Seismological Algorithms*, pp. 89–168, Academic Press, New York, online at "http://sw3d.mff.cuni.cz".

Combescure, M., Ralston, J. & Robert, D. (1999): A proof of the Gutzwiller semiclassical trace formula using coherent state decomposition. *Commun. math. Phys.*, **202**, 463–480.

Kachalov, A.P. (1984): A coordinate system for describing the "quasiphoton" (in Russian). *Zap. Nauchn. Sem. Leningr. Otd. Mat. Instit.*, **140**, 73–76, english transl.: *J. Sov. Math.*, **32**(1986), 151–153.

Klimeš, L. (1984): The relation between Gaussian beams and Maslov asymptotic theory. *Stud. geophys. geod.*, **28**, 237–247, online at "http://sw3d.mff.cuni.cz".

Klimeš, L. (1989): Gaussian packets in the computation of seismic wavefields. *Geophys. J. int.*, **99**, 421–433, online at "http://sw3d.mff.cuni.cz".

Norris, A., White, B.S. & Schreiffer, J.R. (1987): Gaussian wave packets in inhomogeneous media with curved interfaces. *Proc. R. Soc. London*, **A 412**, 93–123.

Ralston, J. (1983): Gaussian beams and the propagation of singularities. In: Littman W. (ed.): *Studies in Partial Differential Equations, MAA Studies in Mathematics, Vol.23*, pp. 206–248, The Math. Assoc. Amer., Washington, DC.

Žáček, K. (2001): Optimization of the shape of Gaussian beams. In: *Seismic Waves in Complex 3-D Structures, Report 11*, pp. 181–201, Dep. Geophys., Charles Univ., Prague, online at "http://sw3d.mff.cuni.cz".

Žáček, K. (2003): Decomposition of the wavefield into optimized Gaussian packets. In: *Seismic Waves in Complex 3-D Structures, Report 13*, pp. 35–43, Dep. Geophys., Charles Univ., Prague, online at "http://sw3d.mff.cuni.cz".