New Approach to Solving the Radiative Transport Equation (Method of Rotated Reference Frames)

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Outline

- Motivation
- Background (spectral methods and RTE)
- RTE in rotated reference frames
- Infinite space
- Slab and boundary conditions
- Application to diffusion tomography
- Conclusions

Motivation

- Diffusion approximation is not accurate in regions with low scattering, near sources or boundaries, in thin samples, etc.
- Under these circumstances, one must use the RTE instead of the DE.
- But RTE is notoriously difficult to solve, especially for highly forward-peaked scattering typically encountered in biological tissues.
- Efficient numerical methods for solving the RTE are needed

Background (Spectral Methods)

Solve system of equations :

$$(z+\mathbf{W})\left|x\right\rangle = \left|b\right\rangle$$

for M different values of z, where

z is a number

$\mathbf{W}$ is an $N\times N$ matrix

$\left|x\right\rangle, \left|b\right\rangle$ are vectors of length N

Spectral method:

1) Diagonalize W (find eigenvectors $\left|n\right\rangle$ and eigenvalues w_n)

2) For every z,

$$\left|x\right\rangle = \sum_{\mathrm{n}} \frac{\left|n\right\rangle\left\langle n|b\right\rangle}{z+w_n}$$

Computational complexity: $N^3 + M\times N^2$

However, if the whole vector $\left|x\right\rangle$ is not needed, the complexity may be as low as

$$N^3 + M\times N$$

Spectral Method for the RTE ?

RTE: $(\hat{\mathbf{s}} \cdot \nabla + \mu_t) I(\mathbf{r}, \hat{\mathbf{s}}) = \mu_s \int P(\hat{\mathbf{s}}, \hat{\mathbf{s}}') I(\mathbf{r}, \hat{\mathbf{s}}') d^2\hat{\mathbf{s}}' + \varepsilon(\mathbf{r}, \hat{\mathbf{s}})$

Where is the "spectral variable" z ?

How can we write this equation in the form $(z + W)\left| I \right\rangle = \left| \varepsilon \right\rangle$?

μ_{t} and μ_{s} do not qualify...

We can try to expand $I(\mathbf{r},\hat{\mathbf{s}})$ into a a 3D Fourier integral with respect to $\mathbf{r}$ and into the basis of ordinary spherical harmonics $Y_{lm}(\theta, \varphi)$ with respect to $\mathbf{s}$ ...

...and see if the equation can be cast into the desired form.

Conventional Method of Spherical Harmonics

This results in the following system of equations with respect to the vector of expansion coefficients $\left|I(\mathbf{k})\right\rangle$ ($\mathbf{k}$ - Fourier variable) :

$$iA^{(x)}k_x\left|I(\mathbf{k})\right\rangle + iA^{(y)}k_y\left|I(\mathbf{k})\right\rangle + iA^{(z)}k_z\left|I(\mathbf{k})\right\rangle + S\left|I(\mathbf{k})\right\rangle = \left|\varepsilon(\mathbf{k})\right\rangle$$

$A^{(x)}$, $A^{(y)}$, $A^{(z)}$ are different matrices.

$$A^{(x)}_{lm,l'm'} = \int \sin\theta \cos\varphi Y^*_{lm}(\theta,\varphi) Y_{l'm'}(\theta,\varphi) \sin\theta d\theta d\varphi \quad , \qquad \text{etc. .....}$$

"This rather awe-inspiring set of equations … has perhaps only academic interest".

K.M.Case, P.F.Zweifel, Linear Transport Theory

Rotated Reference Frames

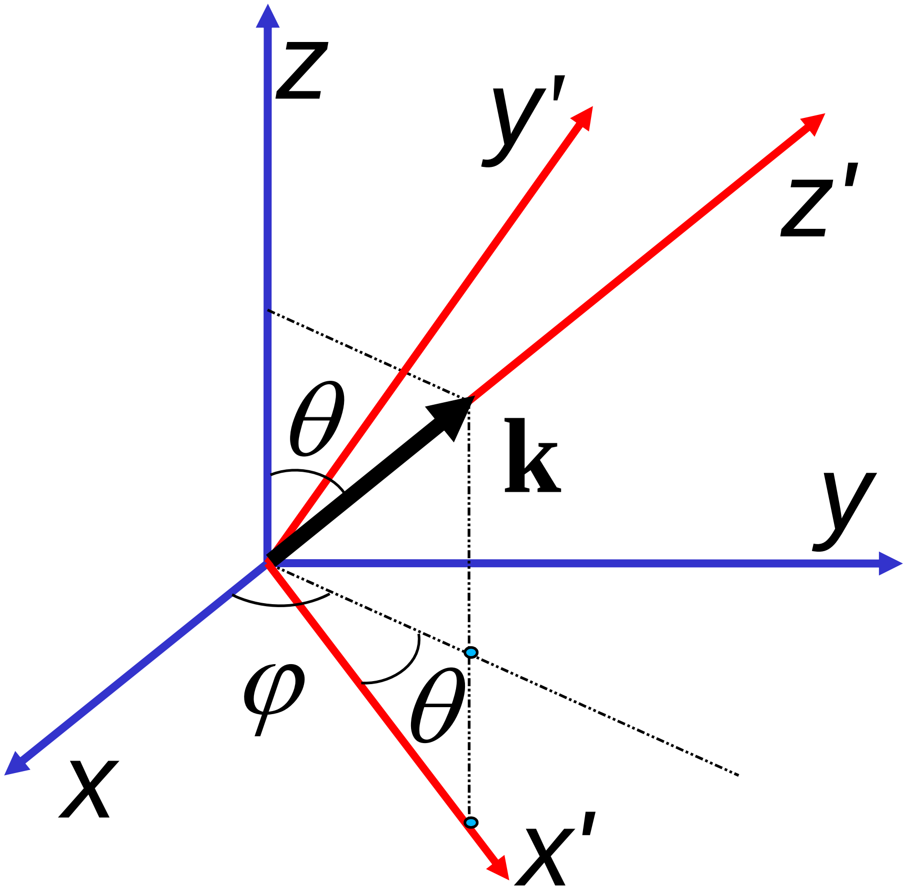
The usual sperical harmonics are defined in the laboratory reference frame. Then θ and φ are the polar angles of the unit vector $\hat{\mathbf{s}}$ in that frame.

THE MAIN IDEA:

For each value of the Fourier variable $\mathbf{k}$, use spherical harmonics defined in a reference frame whose z-axis is aligned with the direction of $\mathbf{k}$.

We call such frames "rotated".
Spherical harmonics defined in the rotaded frame are denoted by $Y(\hat{\mathbf{s}}, \hat{\mathbf{k}})$.

Rotation of the Laboratory Frame (x,y,z).



$$Y_{lm}(\hat{\mathbf{s}},\hat{\mathbf{k}}) = \sum_{m'=-l}^{l} D^{l}_{m'm}(\varphi_k,\theta_k,0)Y_{lm'}(\hat{\mathbf{s}})$$

Wigner D-functions

Euler angles

Spherical functions in the laboratory frame

RTE in the Angular Basis of Rotated Spherical Functions

$$ikA\left|I\right\rangle + S\left|I\right\rangle = \left|\varepsilon\right\rangle$$

Source term

Scalar spectral parameter

Block-tridiagonal real symmetric matrix

Diagonal matrix
$S_{lm,l'm'} = \delta_{ll'}\delta_{mm'}[\mu_a + \mu_s(1 - P_l)]$

Parameters of the phase function. (For the HG model, $P_l = g^l$)

The Spectral Solution

$$I(\mathbf{r},\hat{\mathbf{s}}) = \sum_{l,m} \int \tilde{I}_{lm}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} Y_{lm}(\hat{\mathbf{s}},\hat{\mathbf{k}}) \mathrm{d}^3\mathrm{k} \qquad (1)$$

$$\tilde{I}_{lm}(\mathbf{k}) = \frac{1}{\sqrt{S_l}} \sum_n \frac{\langle lm|\psi_n\rangle\langle\psi_n|\varepsilon\rangle}{1+ik\lambda_n} \qquad (2)$$

Eigenvectors and eigenvalues of a real Symmetric tridiagonal matrix (easy to compute)

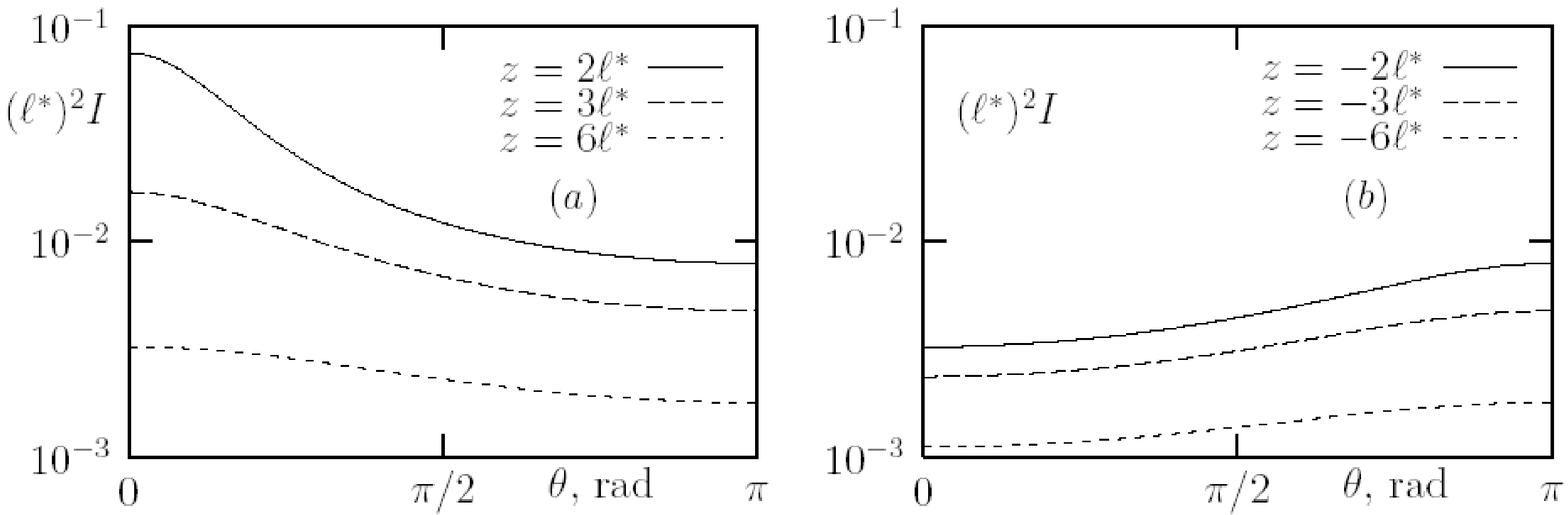
To get the real-space solution, substitute (2) into (1) and compute the integral.

The integral is not easy… but doable.

Details in J.Phys.A 39, 115 (2006)

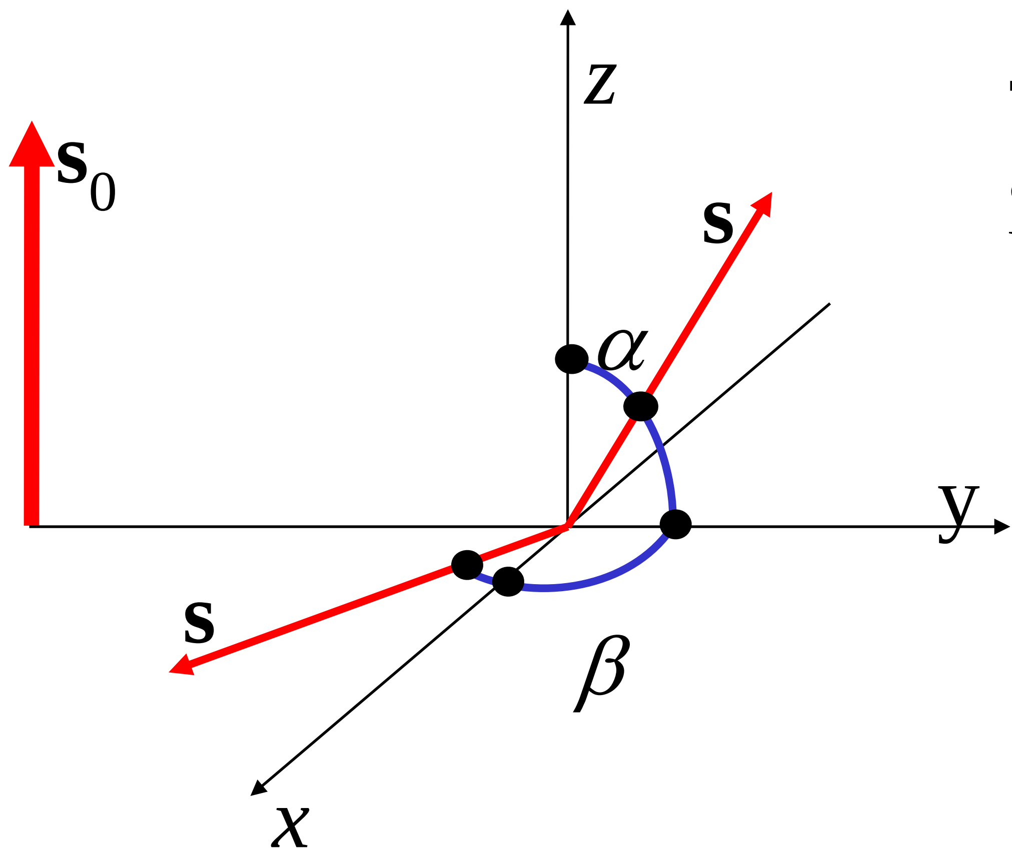
Infinite Space, Point Uni-Directional (Sharply-Peaked) Source

(a) forward and backward propagation



Angular dependence of the specific intensity for forward (a) and backward (b) propagation obtained at $l_{max} = 21$, g = 0.98 and $\mu_a/\mu_s = 6 \cdot 10^{-5}$. The distance to the source z is assumed to be positive for forward propagation and negative for backward propagation.

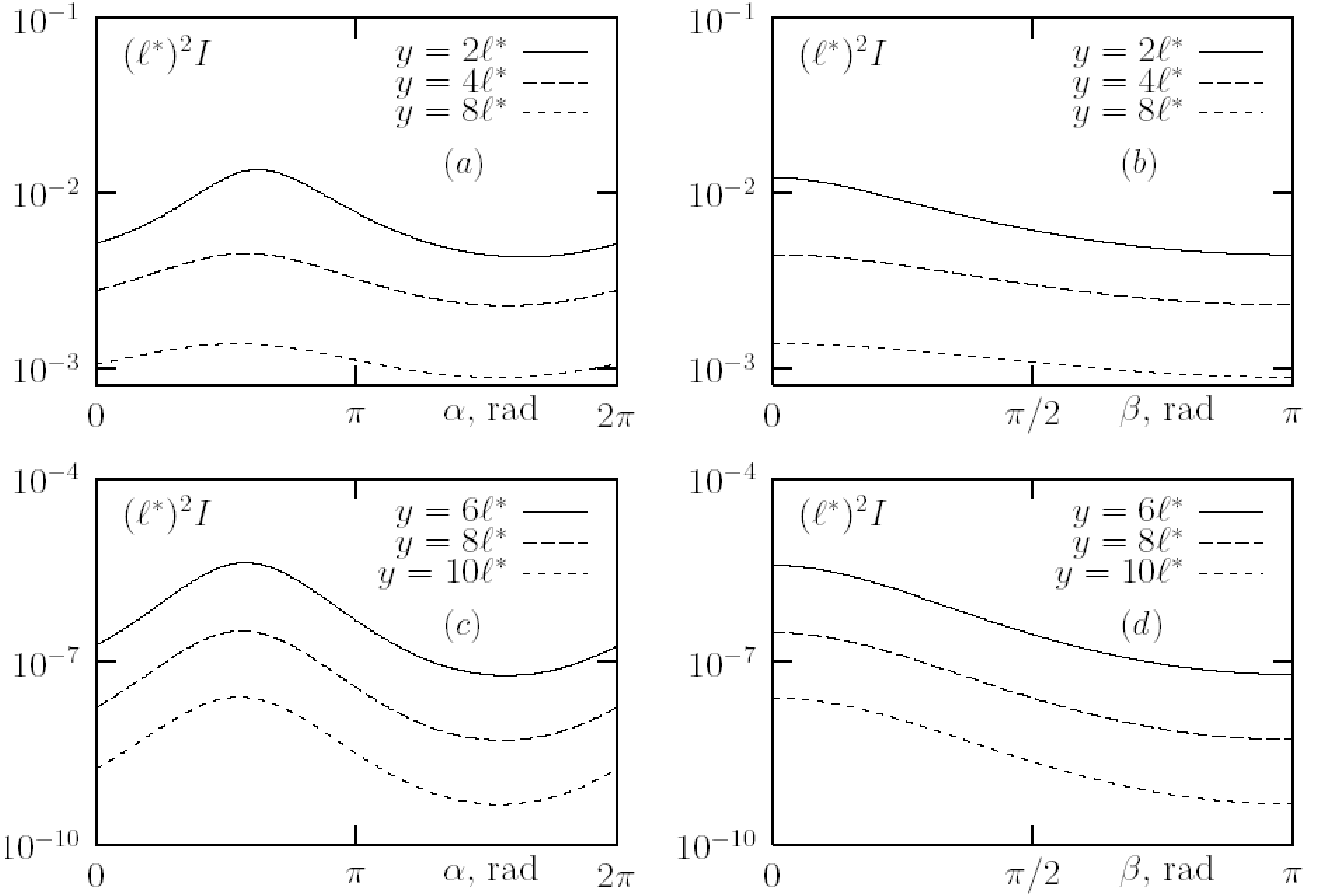
Infinite Space, Point Uni-Directional (Sharply-Peaked) Source
(b) off-axis propagation



Two cases:

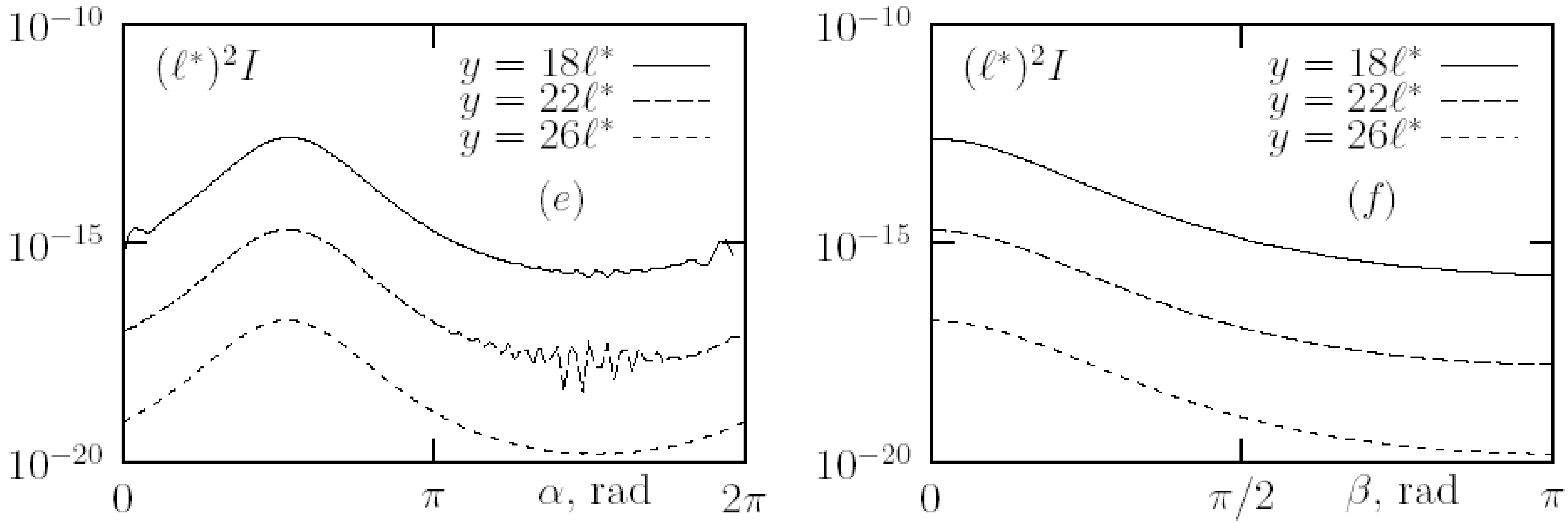
a) **s** is in the xy plane

b) **s** is in the yz plane



Angular distribution of specific intensity for off-axis propagation (relatively small absorption)

Parameters: g = 0.98 and μ_a/μ_s = 6 · 10^{-5} (a), (b), = 0.03 (c), (d).



Angular distribution of specific intensity for off-axis propagation (relatively large absorption)

Parameters: g = 0.98 and $\mu_a/\mu_s = 0.2$.

Evanescent Waves and the BVP in a Slab

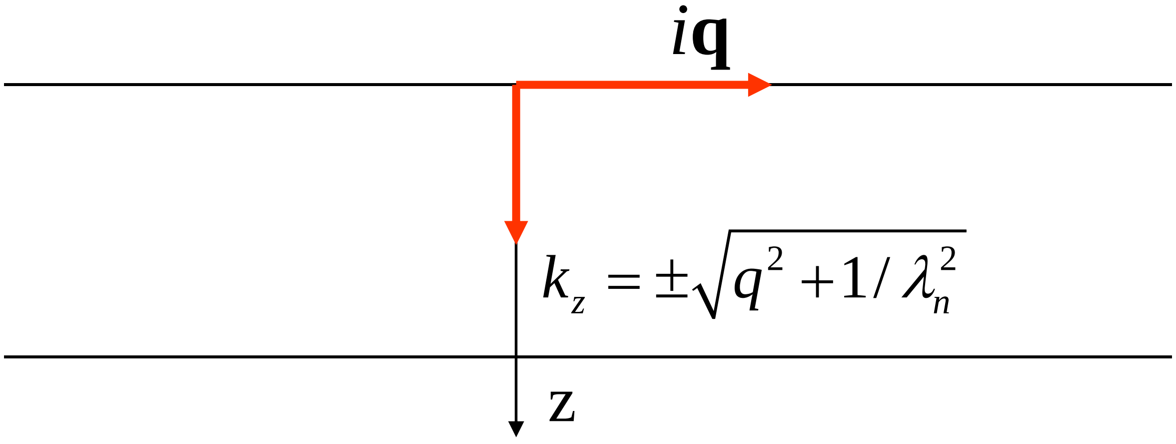
Plane waves:

$$I_{\mathbf{k}} = e^{-\mathbf{k}\cdot\mathbf{r}}\, F_{\mathbf{k}}(\hat{\mathbf{s}}), \qquad |\mathbf{k}| = 1/\lambda_n$$

$$F_{\mathbf{k}}(\hat{\mathbf{s}}) = \sum_{lm} \langle lm | \psi_n \rangle Y_{lm}(\hat{\mathbf{s}}, \hat{\mathbf{k}})$$

Evanescent waves:

$$\mathbf{k} = -i\mathbf{q} \pm \hat{\mathbf{z}}\sqrt{q^2 + 1/\lambda_n^2}, \qquad \mathbf{q}\cdot\hat{\mathbf{z}} = 0$$



Application to Diffusion Tomography in the Slab Imaging Geometry

- This method gives analytical plane-wave expansion of the RTE GF in a slab
- This expansion is needed for fast image reconstruction algorithms that we have recently developed [>10^8 data points in the recent experiment, Z. Wang, G.Y.Panasyuk, V.A.Markel, J.C.Schotland *OL* **30**, 3338 (2005).]
- The method has been developed for constant optical properties. It can be used for ***linearized*** image reconstruction, OR, using the analytical series inversion techniques [V.A.Markel, J.A.O'Sullivan, J.C.Schotland, *JOSA A* **20**, 903 (2003)], even for solving the ***nonlinear*** inverse problem.
- The method has been used to generate forward data in a thin sample [G.Y.Panasyuk, V.A.Markel, and J.C.Schotland, *Applied Physics Letters* **87**, 101111 (2005).]

CONCLUSIONS

- The method of rotated reference frames takes advantage of all symmetries of the RTE (symmetry with respect to rotations and inversions of the reference frame).
- The angular and spatial dependence of the obtained solutions is expressed in terms of analytical functions.
- The analytical part of the solution is of considerable mathematical complexity. This is traded for relative simplicity of the numerical part. We believe that we have reduced the numerical part of the computations to the absolute minimum allowed by the mathematical structure of the RTE

Co-Authors:

George Y. Panasyuk
John C. Schotland

Publications:

1. V.A.Markel, "Modified spherical harmonics method for solving the radiative transport equation," Letter to the Editor, *Waves in Random Media* **14**(1), L13-L19 (2004).

2. G.Y.Panasyuk, J.C.Schotland, and V.A.Markel, "Radiative transport equation in rotated reference frames," *Journal of Physics A*, **39**(1), 115-137 (2006).

3. G.Y.Panasyuk, V.A.Markel, and J.C.Schotland, *Applied Physics Letters **87**, 101111 (2005)*.

Available on the web at
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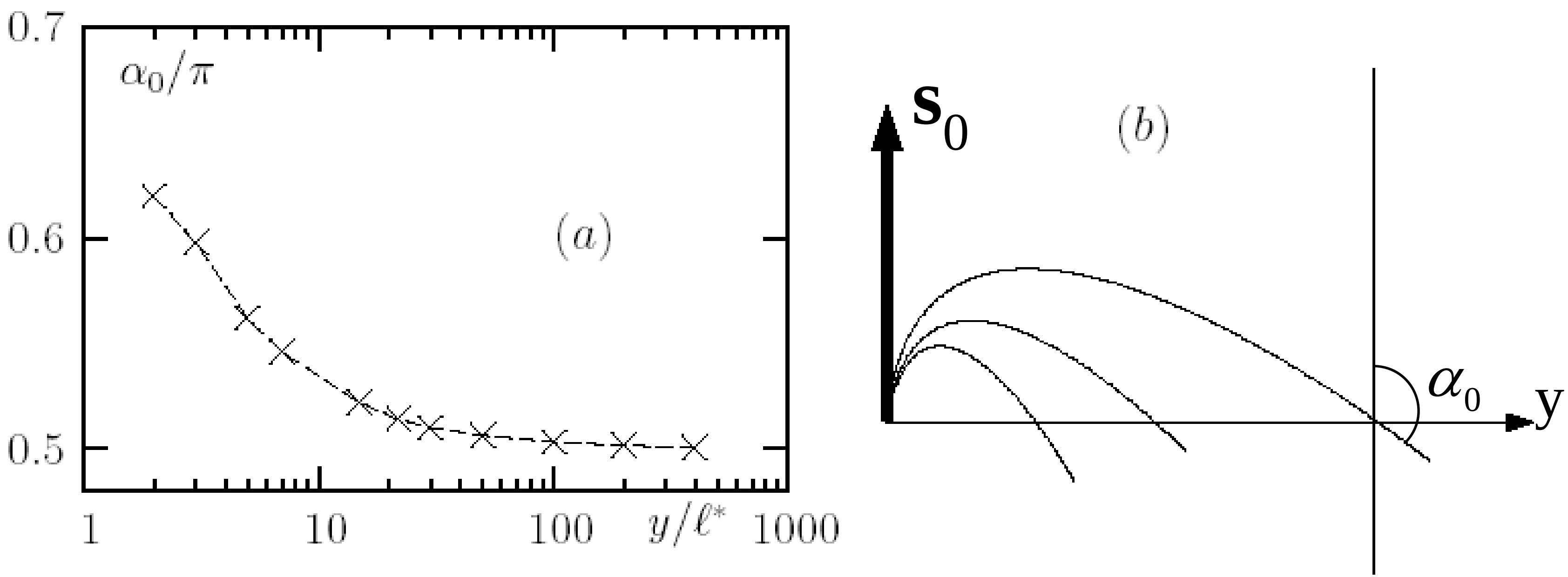

(a) Dependence of the position of maximum α_0 on the distance to the source, y, for physiological parameters: $g = 0.98$ and $\mu_a/\mu_s = 6 \cdot 10^{-5}$.

(b) Schematic illustration of typical "photon trajectories" that correspond to maxima in specific intensity.