Computation of the scattering amplitude in the spheroidal coordinates

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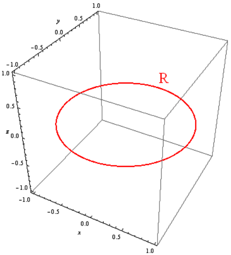
12 October 2015 Lab Seminar
at Kochi University of Technology

Orthogonal curvilinear coordinates

There are several orthogonal curvilinear coordinates in which we can solve the Helmholtz equation by separation of variables.

Today we consider the three-dimensional case, and study the harmonic analysis in the spheroidal coordinates. As an application, we try to calculate the wave functions and the scattering amplitude for the idealized Tonomura model.



Review: Spherical coordinate

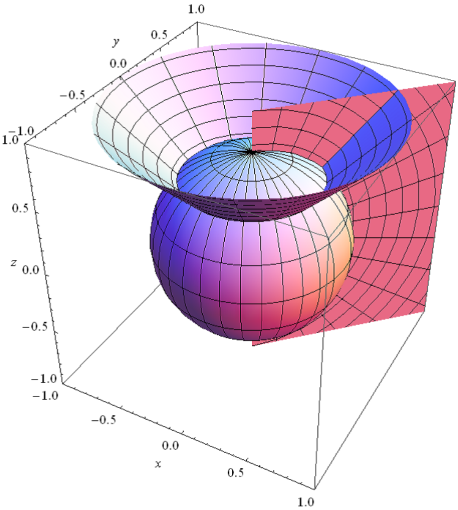
As is well-known, the spherical coordinate in $\mathbb{R}^3$ is defined as follows.

$$\begin{cases} x_1 = r\sin\theta\cos\phi, \\ x_2 = r\sin\theta\sin\phi, \\ x_3 = r\cos\theta, \end{cases} \qquad r \geq 0,\ 0 \leq \eta \leq \pi,\ -\pi < \phi \leq \pi.$$

In the spherical coordinate, the Laplacian is written as

$$\Delta = \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2}{\partial\phi^2}\right].$$

Review: Spherical coordinate



The surface $r = const.$ is a sphere, $\theta = const.$ a cone, $\phi = const.$ a half-plane.

Review: Spherical coordinate

The Helmholtz equation $-\Delta u = k^2 u$ is equivalent to

$$\begin{cases} \dfrac{d^2 f}{dr^2} + \dfrac{2}{r}\dfrac{df}{dr} + \left(k^2 - \dfrac{\ell(\ell+1)}{r^2}\right) f = 0, \\ \dfrac{1}{\sin\theta}\dfrac{d}{d\theta}\left(\sin\theta \dfrac{dg}{d\theta}\right) + \left(\ell(\ell+1) - \dfrac{m^2}{\sin^2\theta}\right) g = 0, \\ \dfrac{d^2 h}{d\phi^2} = -m^2 h, \end{cases}$$

where $u = f(r)g(\theta)h(\phi)$, and ℓ, m are the separation constants.

Review: Spherical coordinate

We have the solutions finite at $r = 0$, $\theta = 0, \pi$, not diverging as $r \to \infty$, and periodic with respect to ϕ, for $\ell = 0, 1, 2, \ldots$, and $m = 0, 1, \ldots, \ell$. The solutions are written as

$$\begin{aligned} u &= j_\ell(kr) P_\ell^m(\cos\theta)\cos(m\phi), \\ u &= j_\ell(kr) P_\ell^m(\cos\theta)\sin(m\phi) \ (m \neq 0). \end{aligned}$$

Here $j_\ell(z) = \sqrt{\pi/(2z)} J_{\ell+1/2}(z)$ is the spherical Bessel function, P_ℓ^m is the associated Legendre function. The number ℓ is called the azimuthal quantum number, and m the magnetic quantum number. The completeness of these solutions are guaranteed by the following formula.

Review: Spherical coordinate

Proposition 1 (Rayleigh's plane wave expansion formula)

Let (r, θ, ϕ) and (k, τ, ψ) are the spherical coordinates for x and p, respectively. That is,

$$\begin{aligned} x &= (r \sin\theta \cos\phi, r \sin\theta \sin\phi, r \cos\theta), \\ p &= (k \sin\tau \cos\psi, k \sin\tau \sin\psi, k \cos\tau). \end{aligned}$$

Then, we have

$$\begin{aligned} e^{ix \cdot p} &= \sum_{\ell=0}^{\infty} \sum_{m=0}^{\ell} \left[i^\ell c_{\ell,m}^2 j_\ell(kr) P_\ell^m(\cos\theta) P_\ell^m(\cos\tau) \cos(m(\phi - \psi)) \right], \\ c_{\ell,m} &= \sqrt{(2 - \delta_{0,m})(2\ell + 1) \frac{(\ell - m)!}{(\ell + m)!}}. \end{aligned}$$

Review: Spherical coordinate

The Fourier inversion formula is described as follows.

$$
\begin{aligned}
u(x) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ix\cdot p} \hat{u}(p)\,dp \\
&= \sum_{\ell=0}^{\infty} \sum_{m=0}^{\ell} i^{\ell} c_{\ell,m} P_{\ell}^{m}(\cos\theta)\cos(m\phi) \int_0^{\infty} j_{\ell}(kr) u_{\ell,m,c}(k) k^2\,dk \\
&\quad + \sum_{\ell=0}^{\infty} \sum_{m=1}^{\ell} i^{\ell} c_{\ell,m} P_{\ell}^{m}(\cos\theta)\sin(m\phi) \int_0^{\infty} j_{\ell}(kr) u_{\ell,m,s}(k) k^2\,dk,
\end{aligned}
$$

$$
\begin{aligned}
u_{\ell,m,c}(k) &= \frac{1}{(2\pi)^{3/2}} \int_{-\pi}^{\pi} \int_0^{\pi} c_{l,m} P_{\ell,m}(\cos\tau)\cos(m\psi)\hat{u}(p)\sin\tau\,d\tau\,d\psi, \\
u_{\ell,m,s}(k) &= \frac{1}{(2\pi)^{3/2}} \int_{-\pi}^{\pi} \int_0^{\pi} c_{l,m} P_{\ell,m}(\cos\tau)\sin(m\psi)\hat{u}(p)\sin\tau\,d\tau\,d\psi.
\end{aligned}
$$

Review: Phase shift and scattering amplitude

Let us explain how to calculate the scattering amplitude for the Schrödinger operator $H = -\Delta + V(r)$ with a radial potential $V(r)$ decaying sufficiently fast at ∞. The free operator $H_0 = -\Delta$ has generalized eigenfunctions with eigenvalue k^2 $(k > 0)$

$$
\begin{aligned}
u &= j_\ell(kr) P_\ell^m(\cos\theta)\cos(m\phi), \\
u &= j_\ell(kr) P_\ell^m(\cos\theta)\sin(m\phi)\ (m \neq 0),
\end{aligned}
$$

and the radial part $j_\ell(kr)$ has the asymptotics

$$
j_\ell(kr) \sim \frac{1}{kr}\cos\left(kr - \frac{(\ell+1)\pi}{2}\right) \quad (r \to \infty).
$$

Review: Phase shift and scattering amplitude

If $V(r)$ decays sufficiently fast at ∞, we can prove that the perturbed operator H has generalized eigenfunctions with eigenvalue k^2 $(k > 0)$

$$u = u_{\ell,k}(r)P_\ell^m(\cos\theta)\cos(m\phi),$$
$$u = u_{\ell,k}(r)P_\ell^m(\cos\theta)\sin(m\phi)\ (m \neq 0)$$

for any $\ell = 0, 1, 2, \dots$ and $m = 0, 1, \dots, \ell$, and $u_{\ell,k}(r)$ has the asymptotics

$$u_{\ell,k}(r) \sim \frac{1}{kr}\cos\left(kr - \frac{(\ell+1)\pi}{2} + \delta_{\ell,k}\right) \quad (r \to \infty),$$

where $\delta_{\ell,k}$ is a real constant called the scattering phase shift.

Review: Phase shift and scattering amplitude

The wave operators $W_\pm$ are defined by

$$W_\pm u = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH} e^{-itH_0} u.$$

Notice that the solution to the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x), \quad \psi(0,x) = u(x)$$

is $\psi(t,x) = e^{-itH}u(x)$. The above definition means the solutions $e^{-itH}W_\pm u$ behave like the free solutions $e^{-itH_0}u$ as $t \to \pm\infty$, respectively.

Review: Phase shift and scattering amplitude

The scattering operator S is defined by $S = W_+^* W_-$. By the conservation of energy, the operator $\mathcal{F} S \mathcal{F}^*$ ($\mathcal{F}$ is the Fourier transform) is decomposed into the direct integral of the operators $S(E)$ ($E > 0$) acting on $L^2(S_E)$, where S_E is the energy shell

$$S_E = \{\xi \in \mathbb{R}^3 \mid |\xi|^2 = E\} = \{\sqrt{E}\omega \mid \omega \in S^2\}.$$

Then the scattering amplitude $f(k^2; \omega, \omega')$ is defined by the formula

$$(S(k^2) - I)(\omega, \omega') = \frac{ki}{2\pi} f(k^2; \omega, \omega') \quad (\omega, \omega' \in S^2).$$

The quantity $|f(k^2; \omega, \omega')|^2$ is called the differential scattering cross section, which is proportional to the ratio of the particles with energy k^2, incident direction ω' and final direction ω.

Review: Phase shift and scattering amplitude

Proposition 2 (Formula for the scattering amplitude)

Given the scattering phase shifts $\delta_{\ell,k}$, the scattering amplitude for the whole operator is given by

$$
\begin{aligned}
& f(k^2;\omega,\omega') \\
= \; & \frac{1}{2ik}\sum_{\ell=0}^{\infty}(e^{2i\delta_{\ell,k}}-1)\sum_{m=0}^{\ell} c_{\ell,m}^2 P_\ell^m(\cos\theta)P_\ell^m(\cos\tau)\cos(m(\phi-\psi)) \\
= \; & \sum_{\ell=0}^{\infty}\frac{e^{2i\delta_{\ell,k}}-1}{2ik}(2\ell+1)P_\ell(\omega\cdot\omega').
\end{aligned}
$$

The final result depends only on the angle between ω and ω', because of the spherical symmetry of the system (V is radial).

Review: Phase shift and scattering amplitude

In summary,

(1) By the spherical coordinate, we can decompose the scattering problem in the three-dimensional space to the problem in the one-dimensional space (scattering phase shift).

(2) By using the plane wave expansion formula, we can sum up the partial scattering data and get the scattering amplitude for the whole operator.

This machinery also works in the case of the spheroidal coordinate. There are two spheroidal coordinates (the prolate spheroidal coordinate and the oblate spheroidal coordinate), but today we only use the oblate one.

Oblate spheroidal coordinate

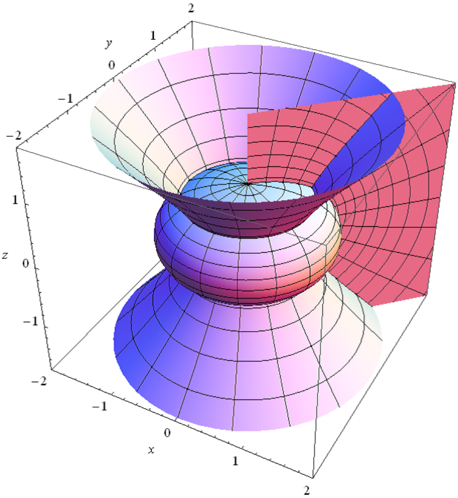
The oblate spheroidal coordinate is defined as follows.

$$\begin{cases} x_1 = a\cosh\xi\sin\eta\cos\phi, \\ x_2 = a\cosh\xi\sin\eta\sin\phi, \\ x_3 = a\sinh\xi\cos\eta, \end{cases}$$

$$\xi \geq 0,\ 0 \leq \eta \leq \pi,\ -\pi < \phi \leq \pi,$$

where a is a positive constant. This definition is taken from 'Iwanami mathematical formulas III' (there is another formulation).

Oblate spheroidal coordinate



The surface $\xi = const.$ is a flattened ellipsoid, $\eta = const.$ a hyperboloid of one sheet, $\phi = const.$ a half-plane.

Laplacian in the oblate spheroidal coordinate

The Laplacian is written as follows.

$$\begin{aligned}\Delta u &= \frac{1}{a^2 \cosh\xi \sin\eta (\cosh^2\xi - \sin^2\eta)} \\ &\cdot \left(\sin\eta \frac{\partial}{\partial\xi}\left(\cosh\xi \frac{\partial u}{\partial\xi}\right) + \cosh\xi \frac{\partial}{\partial\eta}\left(\sin\eta \frac{\partial u}{\partial\eta}\right) \right. \\ &\left. + \frac{\cosh^2\xi - \sin^2\eta}{\cosh\xi \sin\eta} \frac{\partial^2 u}{\partial\phi^2} \right).\end{aligned}$$

If we put $u = f(\xi)g(\eta)h(\phi)$, the Helmholtz equation $-\Delta u = k^2 u$ is reduced to the following ordinary differential equations.

Laplacian in the oblate spheroidal coordinate

$$
\begin{aligned}
&\frac{1}{\cosh\xi}\frac{d}{d\xi}\left(\cosh\xi\frac{df}{d\xi}\right) \\
&\qquad + \left(a^2k^2\cosh^2\xi - \mu + \frac{m^2}{\cosh^2\xi}\right)f = 0, && (1) \\
&\frac{1}{\sin\eta}\frac{d}{d\eta}\left(\sin\eta\frac{dg}{d\eta}\right) \\
&\qquad + \left(-a^2k^2\sin^2\eta + \mu - \frac{m^2}{\sin^2\eta}\right)g = 0, && (2) \\
&\frac{d^2h}{d\phi^2} = -m^2h. && (3)
\end{aligned}
$$

Here m, μ are the separation constants.

Laplacian in the oblate spheroidal coordinate

We require

(a) $g(\eta)$ is finite at $\eta = 0, \pi$,

(b) $h(\phi)$ has period 2π, and

(c) u is single-valued with respect to the original coordinate x.

By (b) and (3), we have

$$h(\phi) = \cos(m\phi) \ (m = 0, 1, 2, \ldots),$$
$$h(\phi) = \sin(m\phi) \ (m = 1, 2, \ldots).$$

Laplacian in the oblate spheroidal coordinate

We put $\lambda = \mu - a^2k^2$, $c = -iak$. By the change of variable $z = i\sinh\xi$ in (1), and $w = \cos\eta$ in (2), we have

$$\frac{d}{dz}\left((1-z^2)\frac{df}{dz}\right) + \left(\lambda - c^2z^2 - \frac{m^2}{1-z^2}\right) f = 0, \tag{4}$$
$$\frac{d}{dw}\left((1-w^2)\frac{dg}{dw}\right) + \left(\lambda - c^2w^2 - \frac{m^2}{1-w^2}\right) g = 0. \tag{5}$$

Thus the two equations (4) and (5) are equivalent as equations for complex variables. Especially when $c = 0$, these equations become the associated Legendre differential equation, which is obtained from the equation for $g(\theta)$ in the spherical coordinate by the change of variable $w = \cos\theta$.

Angular spheroidal wave function

By the requirement (a), we need the solutions to (5) finite at $w = \pm 1$. For fixed $m = 0, 1, 2, \ldots$, there are at most countable values of λ's for which the equation (5) has a non-trivial solution finite at $w = \pm 1$. We denote such values by

$$\lambda_{m\ell} \quad (\ell = m, m+1, m+2, \ldots),$$

and corresponding solutions by $S_{m\ell}(c, w)$. We call $S_{m\ell}(c, w)$ the angular spheroidal wave function (of the first kind) . When $c = 0$, $S_{m\ell}(0, w)$ coincides with the associated Legendre function $P_\ell^m(w)$. $S_{m\ell}(c, w)$ is normalized as

$$\int_{-1}^{1} |S_{m\ell}(c, w)|^2 dw = \frac{2}{2\ell+1} \frac{(\ell+m)!}{(\ell-m)!}.$$

Radial spheroidal wave function

Notice that $S_{m\ell}(c,z)$ is also a solution to the radial equation (4) with the same parameter $\lambda = \lambda_{m\ell}$. We introduce another solution $R^{(1)}_{m\ell}(c,z)$, which is a constant multiple of $S_{m\ell}(c,z)$, and behaves like

$$R^{(1)}_{m\ell}(c,z) \sim \frac{1}{cz}\cos\left(cz - \frac{\ell+1}{2}\pi\right) \quad \text{as} \quad z \to i\infty. \tag{6}$$

Notice that $z \to i\infty$ corresponds the limit $\xi \to \infty$, and

$$cz = -iak \cdot i\sinh\xi = k \cdot a\sinh\xi \sim kr \quad (\xi \to \infty).$$

Thus (6) means $R^{(1)}_{m\ell}(c,z)$ behaves like usual spherical Bessel function at infinity. We call $R^{(1)}_{m\ell}(c,z)$ the radial spheroidal wave function of the first kind.

Radial spheroidal wave function

Notice that the left hand side of the equation (4) preserves the parity of f. Actually, $R^{(1)}_{m\ell}(c,z)$ is an even function if $\ell - m$ is even, and an odd function if $\ell - m$ is odd (the same as $P^m_\ell(z)$). Then, there exists a non-trivial solution to (4) which has the opposite parity to that of $R^{(1)}_{m\ell}(c,z)$. We denote such solution by $R^{(5)}_{m\ell}(c,z)$ ($R^{(j)}_{m\ell}(c,z)$ for $j = 2,3,4$ are already defined in the handbook of Abramowitz and Stegun). We normalize $R^{(5)}_{m\ell}(c,z)$ so that there exists a constant $\delta^m_{\ell,k}$ such that

$$R^{(5)}_{m\ell}(c,z) \sim \frac{1}{cz}\cos\left(cz - \frac{\ell+1}{2}\pi + \delta^m_{\ell,k}\right) \quad \text{as} \quad z \to i\infty. \tag{7}$$

Matching condition

Let us consider the requirement (c). Notice that in the spheroidal coordinate

$$\begin{cases} x_1 = a\cosh\xi\sin\eta\cos\phi, \\ x_2 = a\cosh\xi\sin\eta\sin\phi, \\ x_3 = a\sinh\xi\cos\eta, \end{cases}$$

the two coordinates (ξ, η, ϕ) and $(-\xi, \pi-\eta, \phi)$ give the same point x. Thus (c) implies

$$f(\xi)g(\eta) = f(-\xi)g(\pi-\eta).$$

Since $z = i\sinh\xi$ and $w = \cos\eta$, the above condition requires f and g have the same parity with respect to z and w, respectively.

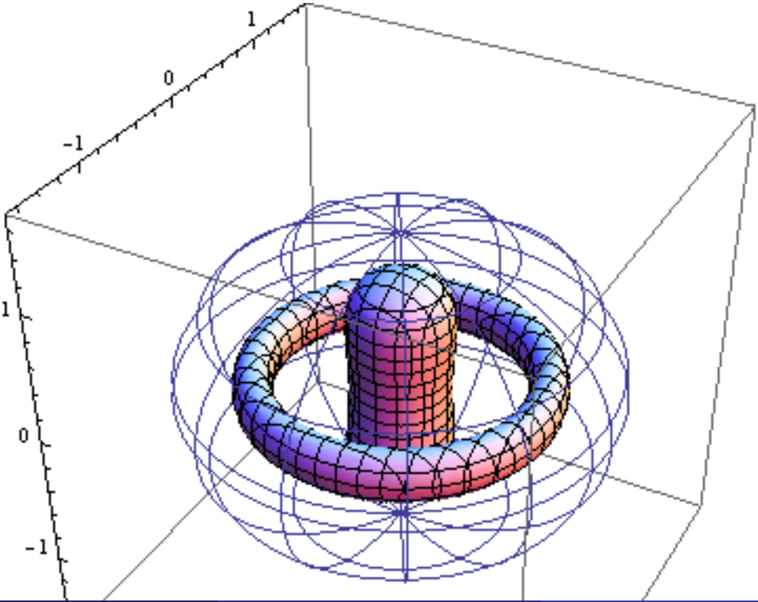
The generalized eigenfunctions for $-\Delta$

In summary, we obtain generalized eigenfunctions for $-\Delta$ with eigenvalue k^2

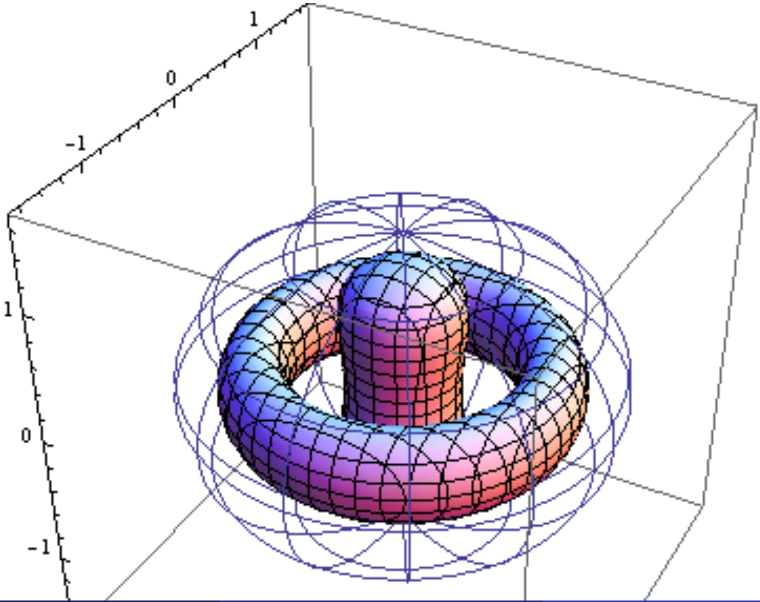
$$
\begin{aligned}
&u = S_{m\ell}(-iak, i\sinh\xi)R^{(1)}_{m\ell}(-iak, \cos\eta)\cos m\phi, \\
&u = S_{m\ell}(-iak, i\sinh\xi)R^{(1)}_{m\ell}(-iak, \cos\eta)\sin m\phi, \\
&m = 0, 1, 2, \dots, \\
&\ell = m, m+1, m+2, \dots.
\end{aligned}
$$

As an application, we give some level surfaces of an eigenfunction for $-\Delta$ in a flattened ellipsoid with the Dirichlet boundary conditions.

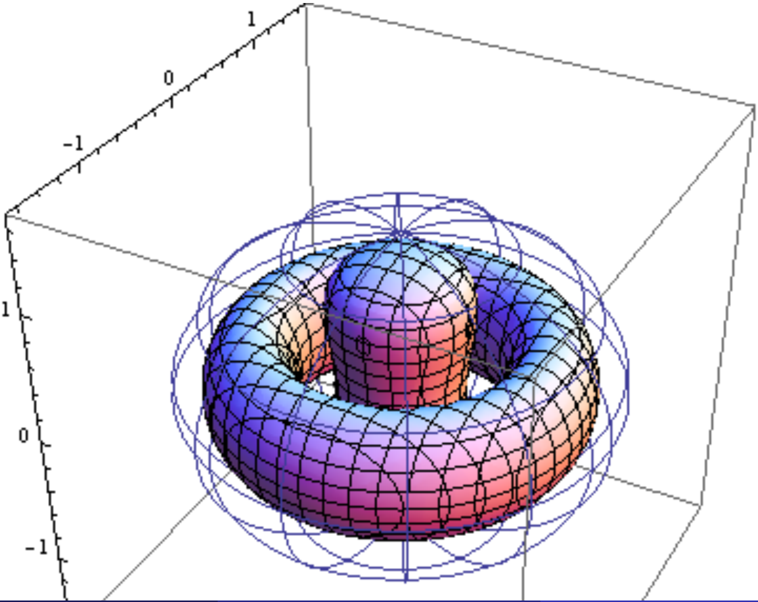
Level surfaces of a Dirichlet eigenfunction



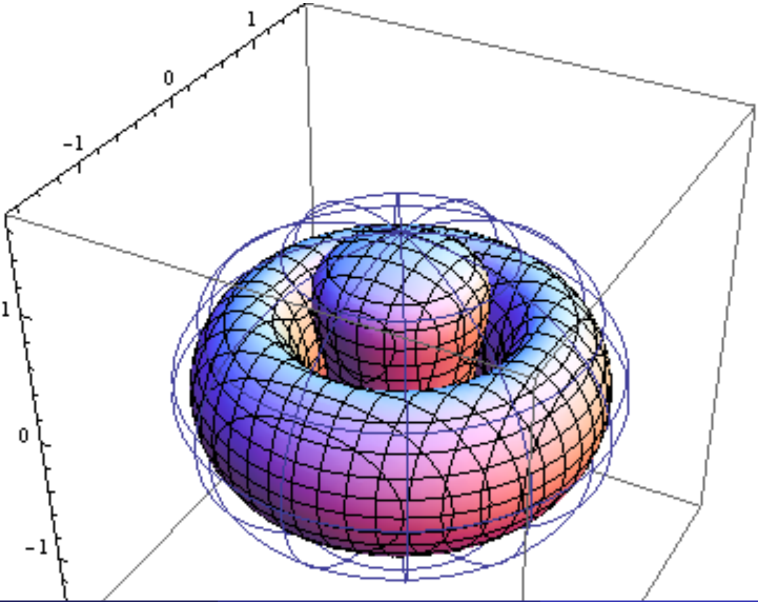
Level surfaces of a Dirichlet eigenfunction



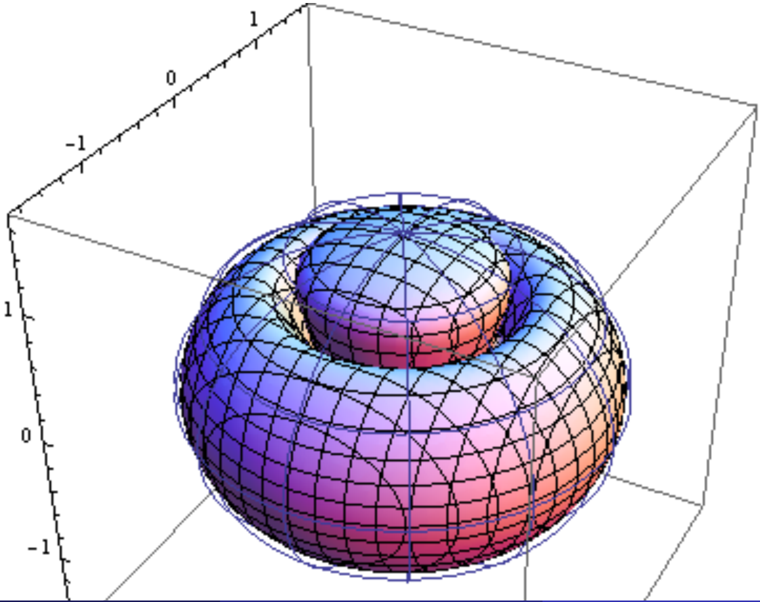
Level surfaces of a Dirichlet eigenfunction



Level surfaces of a Dirichlet eigenfunction



Level surfaces of a Dirichlet eigenfunction

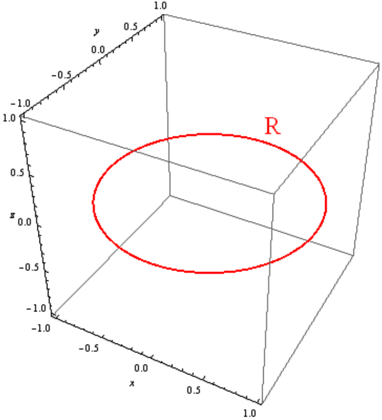


Idealized Tonomura model

We consider a ring in $\mathbb{R}^3$,

$$R = \{x \in \mathbb{R}^3 \mid |x| = a,\ x_3 = 0\}$$

in which a quantized magnetic flux is enclosed. This is an idealized model to the experiment by Tonomura et al. Actually, we can obtain the explicit generalized eigenfunctions for this model, by using the oblate spheroidal coordinate.



Idealized Tonomura model

The corresponding Hamiltonian is

$$H = \left(\frac{1}{i}\nabla \ - A\right)^2 \quad \text{on} \quad \mathbb{R}^3,$$

where $A \in C^\infty(\mathbb{R}^3 \setminus R; \mathbb{R}^3)$ is the magnetic vector potential satisfying

$$\nabla \times A = 0 \quad \text{in} \quad \mathbb{R}^3 \setminus R,$$
$$\int_D (\nabla \times A) \cdot n\, dS = \int_{\partial D} A \cdot d\ell = \pi$$

for any small disc D pierced by the ring R, where n is the unit normal vector on D (the direction of n is appropriately fixed). Actually we can take A satisfying the above conditions and the support A is bounded in $\mathbb{R}^3$ (we assume this condition below).

Idealized Tonomura model

Take $x_0 \in \mathbb{R}^3$ sufficiently large, and consider a phase function defined by the line integral

$$\Phi(x) = \exp\left(i \int_{x_0}^{x} A \cdot d\ell\right).$$

The function Φ is two-valued, since

$$\exp\left(i \int_{\partial D} A \cdot d\ell\right) = e^{i\pi} = -1$$

for any small disc D pierced by R. Moreover,

$$\Phi\left(\frac{1}{i}\nabla\right)\Phi^{-1} u = \left(\frac{1}{i}\nabla - A\right) u.$$

Idealized Tonomura model

Thus we have the intertwining relation

$$Hu = \Phi(-\Delta)\Phi^{-1}u.$$

We put $v = \Phi^{-1}u$. Then,

$$Hu = k^2 u \Leftrightarrow -\Delta v = k^2 v,$$

which is the Helmholtz equation. But v is a two-valued function in the sense that $v(x)$ changes the sign when x moves along an edge of a small disc pierced by the ring R.

Idealized Tonomura model

We need the solution for $-\Delta v = k^2 v$, by putting $v = f(\xi)g(\eta)h(\phi)$. The equations for f, g, h are the same as before, but we require

(a) $g(\eta)$ is finite at $\eta = 0, \pi$,

(b) $h(\phi)$ has period 2π, and

(c)' $v(x)$ changes the sign when x moves along an edge of a small disc pierced by the ring R.

The requirement (c)' is equivalent to the condition

$$f(\xi)g(\eta) = -f(-\xi)g(\pi - \eta).$$

Thus f and g have opposite parities with respect to z and w, respectively.

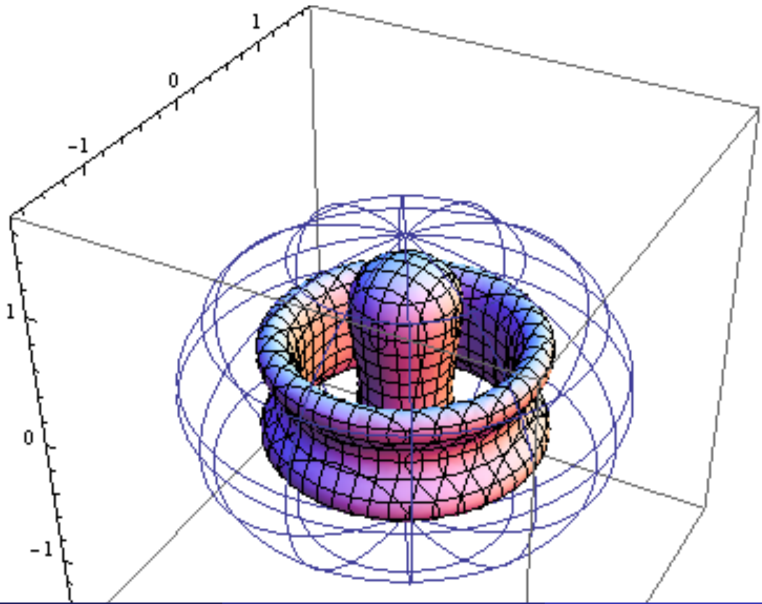
Idealized Tonomura model

In summary, H has generalized eigenfunctions with energy k^2

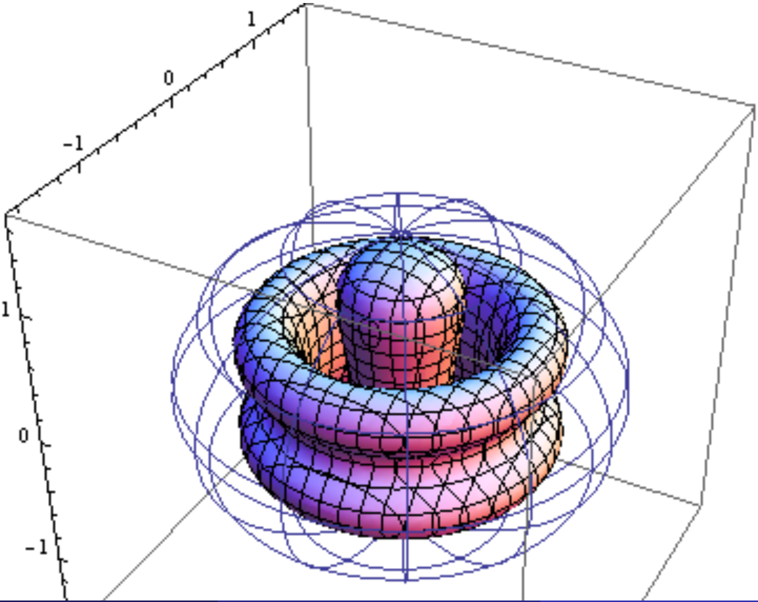
$$
\begin{aligned}
&u = \Phi \cdot S_{m\ell}(-iak, i\sinh\xi) R^{(5)}_{m\ell}(-iak, \cos\eta) \cos m\phi, \\
&u = \Phi \cdot S_{m\ell}(-iak, i\sinh\xi) R^{(5)}_{m\ell}(-iak, \cos\eta) \sin m\phi, \\
&m = 0, 1, 2, \ldots, \\
&\ell = m, m+1, m+2, \ldots.
\end{aligned}
$$

As an application, we give some level surfaces for an eigenfunction of H in a flattened ellipsoid with Dirichlet boundary conditions.

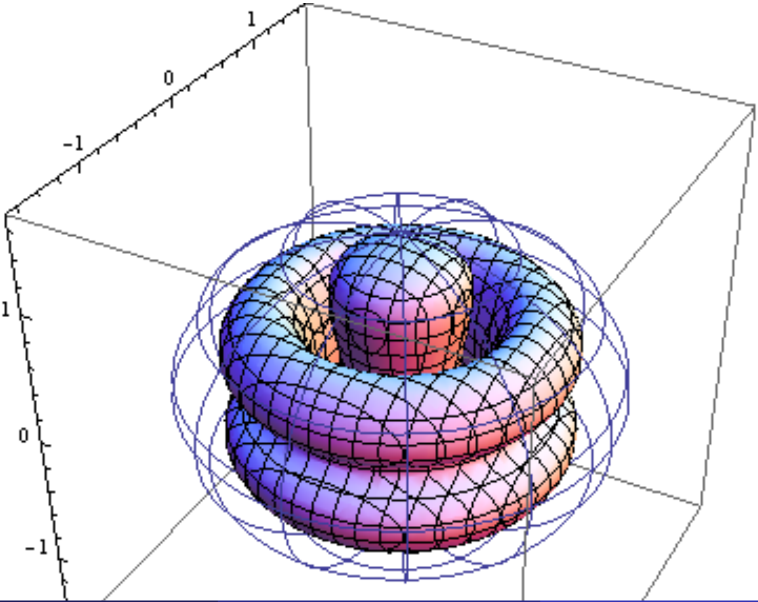
Level surfaces of a Dirichlet eigenfunction for H



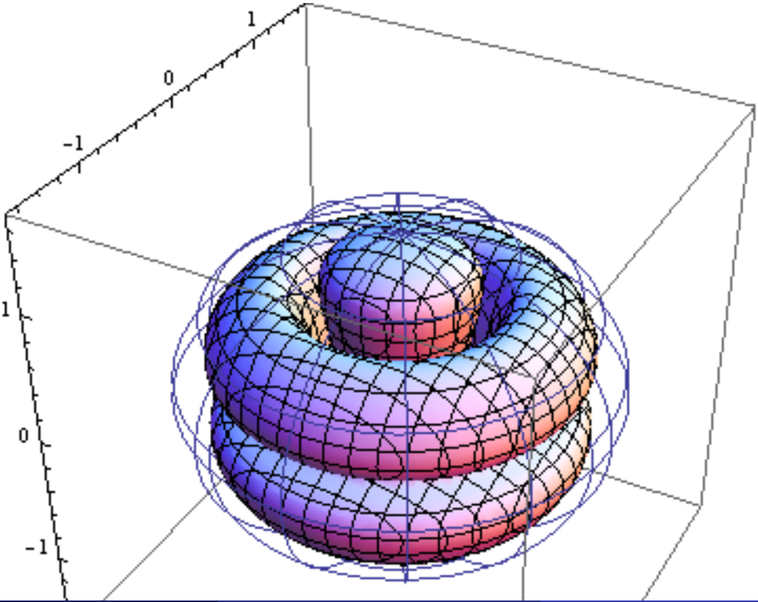
Level surfaces of a Dirichlet eigenfunction for H



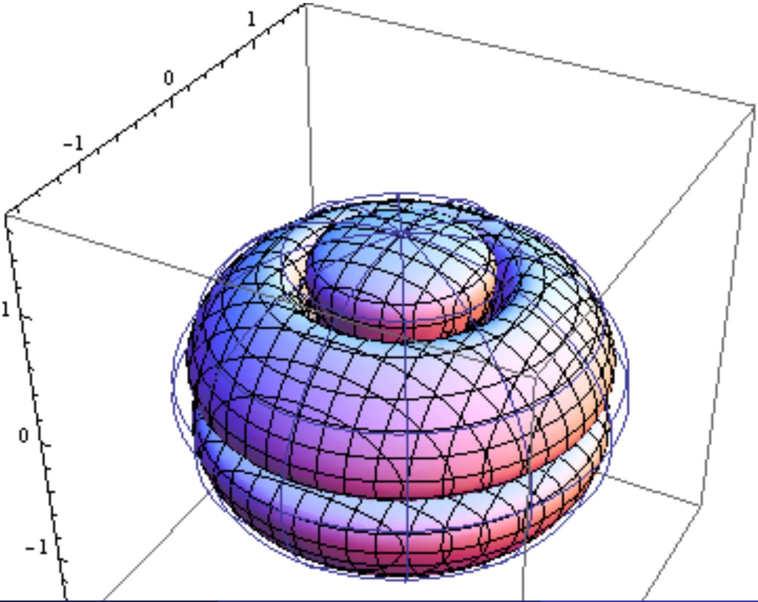
Level surfaces of a Dirichlet eigenfunction for H



Level surfaces of a Dirichlet eigenfunction for H



Level surfaces of a Dirichlet eigenfunction for H



Plane wave expansion formula

In order to develop the scattering theory, we use the plane wave expansion formula in spheroidal coordinate, which is given in the Flammer's book.

Proposition 3

We use the oblate spheroidal coordinate in x-space and the spherical coordinate in p-space, that is,

$$\begin{cases} x_1 = a\cosh\xi\sin\eta\cos\phi, \\ x_2 = a\cosh\xi\sin\eta\sin\phi, \\ x_3 = a\sinh\xi\cos\eta, \end{cases} \qquad \begin{cases} p_1 = k\sin\tau\cos\psi, \\ p_2 = k\sin\tau\sin\psi, \\ p_3 = k\cos\tau. \end{cases}$$

Plane wave expansion formula

Proposition (continued)

Then, we have

$$e^{ix\cdot p} = \sum_{m=0}^{\infty}\sum_{\ell=m}^{\infty} i^{\ell} c_{\ell,m}^2 R_{m\ell}^{(1)}(-iak, i\sinh\xi) \cdot S_{m\ell}(-iak,\cos\eta) S_{m\ell}(-iak,\cos\tau)\cdot\cos m(\phi-\psi).$$

Here, the normalization constants $c_{\ell,m}$ is the one in the Rayleigh's formula.

Notice that $R_{m\ell}^{(1)}(-iak, i\sinh\xi)$ and $j_\ell(kr)$ has the same asymptotics as $\xi\to\infty$ $(r\to\infty)$.

Scattering theory in the spheroidal coordinate

Remind that the phase shifts $\delta^m_{\ell,k}$ are introduced as follows.

$$
\begin{aligned}
R^{(1)}_{m\ell}(-iak, i\sinh\xi) &\sim \frac{1}{kr}\cos\left(kr - \frac{(\ell+1)\pi}{2}\right), \\
R^{(5)}_{m\ell}(-iak, i\sinh\xi) &\sim \frac{1}{kr}\cos\left(kr - \frac{(\ell+1)\pi}{2} + \delta^m_{\ell,k}\right),
\end{aligned}
$$

as $r \to \infty$. In this case, $\delta^m_{\ell,k}$ depends on both ℓ and m (in the case of radial V, it depends only on ℓ). Then the scattering amplitude is calculated as follows.

Scattering theory in the spheroidal coordinate

Theorem 1

We introduce the spherical coordinate (τ, ψ) *in* S^2 *as*

$$\omega = (\sin\tau\cos\psi, \sin\tau\sin\psi, \cos\tau),$$
$$\omega' = (\sin\tau'\cos\psi', \sin\tau'\sin\psi', \cos\tau').$$

Then, the scattering amplitude with energy k^2 *for the pair* H *and* $H_0 = -\Delta$ *is*

$$\begin{aligned} & f(k^2;\omega,\omega') \\ = \; & \frac{1}{2ik}\sum_{m=0}^{\infty}\sum_{\ell=m}^{\infty}(e^{2i\delta_{\ell,k}^m}-1)c_{\ell,m}^2 \\ & \cdot S_{m\ell}(-iak,\cos\tau)S_{m\ell}(-iak,\cos\tau')\cos(m(\phi-\psi)). \end{aligned}$$

Numerical calculation of the scattering wave

The plane wave expansion formula is also useful in the calculation of the plane wave scattered by the Tonomura ring. The incident plane wave with momentum p in the perturbed system is described as

$$\begin{aligned} W_- e^{ix\cdot p} \;&=\; \Phi \cdot \sum_{m=0}^{\infty}\sum_{\ell=m}^{\infty} i^{\ell} c_{\ell,m}^{2} e^{i\delta_{\ell,k}^{m}} R_{m\ell}^{(5)}(-iak, i\sinh\xi) \\ &\quad \cdot S_{m\ell}(-iak,\cos\eta) S_{m\ell}(-iak,\cos\tau) cos(m(\phi-\psi)), \end{aligned}$$

where Φ is the (two-valued) gauge function used in the construction of the vector potential A.

Numerical calculation of the scattering wave

There is ambiguity of the choice of the gauge function Φ. For simplicity, we take $\Phi = 1$, then the wave function satisfies the boundary condition

$$
\begin{aligned}
u(x_1, x_2, +0) &= -u(x_1, x_2, -0), \\
\frac{\partial u}{\partial x_3}(x_1, x_2, +0) &= -\frac{\partial u}{\partial x_3}(x_1, x_2, -0)
\end{aligned}
$$

for $x_1^2 + x_2^2 < a^2$. Thus the wave function might have discontinuity on the disc enclosed by the ring R. In the real experiment, we can observe only the square of the absolute value of the wave function, as the hitting probability of the scattered particles. So, this is not essential.

Numerical calculation of the scattering wave

According to the numerical calculation, the phase shift $\delta^m_{\ell,k}$ decays very rapidly as $\ell \to \infty$. If $\delta^m_{\ell,k}$ is very small, then we have

$$e^{i\delta^m_{\ell,k}} R^{(5)}_{m\ell}(-iak, i\sinh\xi) \sim R^{(1)}_{m\ell}(-iak, i\sinh\xi).$$

Taking the difference with the usual plane wave expansion, we have

$$\begin{aligned} & W_- e^{ix\cdot p} \\ \sim \; & e^{ix\cdot p} + \sum_{\delta^m_{\ell,k}:\ \text{not small}} i^\ell c^2_{\ell,m} \left(e^{i\delta^m_{\ell,k}} R^{(5)}_{m\ell} - R^{(1)}_{m\ell} \right) (-iak, i\sinh\xi) \\ & \cdot S_{m\ell}(-iak, \cos\eta) S_{m\ell}(-iak, \cos\tau) cos(m(\phi - \psi)). \end{aligned}$$

This approximation can greatly unburden the numerical calculation.

Numerical calculation of the scattering wave

For the calculation of the phase shift $\delta^m_{\ell,k}$, we need another spheroidal function $R^{(2)}_{m\ell}(c,z)$, which has the asymptotics

$$R^{(2)}_{m\ell}(c,z) \sim \frac{1}{cz} \sin\left(cz - \frac{\ell+1}{2}\pi\right) \quad \text{as} \quad z \to i\infty.$$

Then we have

$$R^{(5)}_{m\ell}(c,z) = \cos(\delta^m_{\ell,k}) R^{(1)}_{m\ell}(c,z) - \sin(\delta^m_{\ell,k}) R^{(2)}_{m\ell}(c,z),$$

$$\delta^m_{\ell,k} = \begin{cases} \arctan\left(R^{(1)}_{m\ell}(c,0)/R^{(2)}_{m\ell}(c,0)\right) & (l-m\text{: even}), \\ \arctan\left((R^{(1)}_{m\ell})'(c,0)/(R^{(2)}_{m\ell})'(c,0)\right) & (l-m\text{: odd}). \end{cases}$$

Numerical calculation of the scattering wave

Fortunately, Wolfram Mathematica knows how to calculate $R^{(1)}_{m\ell}$ and $R^{(2)}_{m\ell}$. We give here the tables of $|e^{i\delta^m_{\ell,k}} - 1|$ for several l and m, in the case $a = 1$ and $k = 1$.

$l \backslash m$	0	1	2	3
0	0.610919	-	-	-
1	0.079627	0.105036	-	-
2	0.001266	0.001833	0.006314	-
3	0.000009	0.000012	0.000029	0.000163

Table: $|e^{i\delta^m_{\ell,k}} - 1|$ for $a = 1$ and $k = 1$.

Thus, taking only the term for $(\ell, m) = (0, 0)$ is not so bad approximation.

Numerical calculation of the scattering wave

We assume $a = 1$ and the incident direction is x_1-direction ($p = (1, 0, 0)$), so $k = 1$, $\tau = \pi/2$, $\psi = 0$. The approximation of the incident plane wave is

$$\begin{aligned} W_- e^{ix_1} &\sim e^{ix_1} + c^2_{0,0}\left(e^{i\delta^0_{0,1}} R^{(5)}_{00} - R^{(1)}_{00}\right)(-i, i\sinh\xi) \\ &\quad \cdot S_{00}(-i, \cos\eta) S_{00}(-i, 0). \end{aligned}$$

From the next page, we shall exhibit the time propagation of the incident plane wave, by plotting the imaginary part of the wave function on xy-plane and xz-plane.

Time propagation of the horizontal plane wave

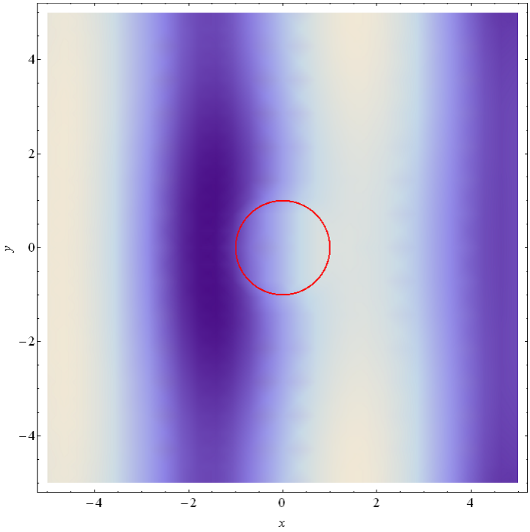
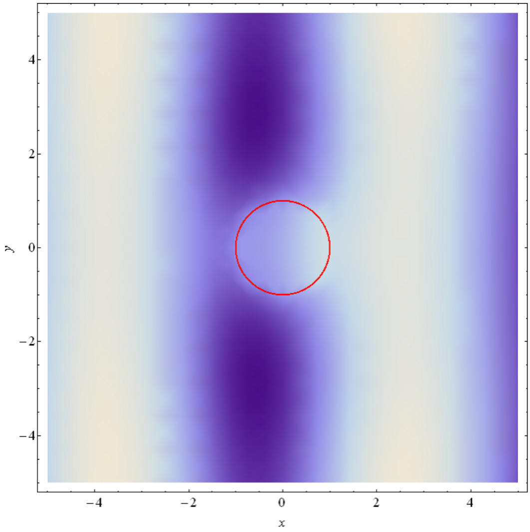


Figure: The imaginary part of the incident plane wave on xy-plane.

Time propagation of the horizontal plane wave



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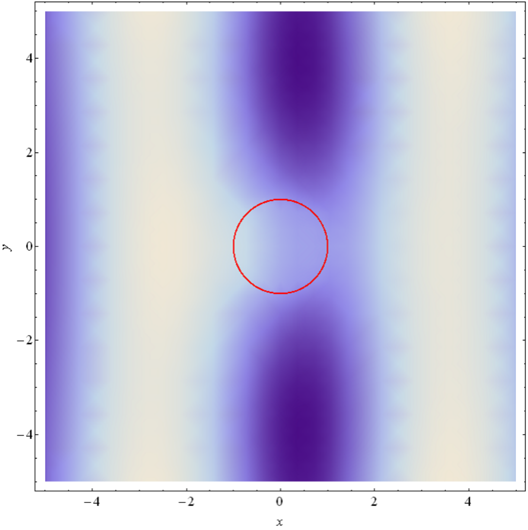
Time propagation of the horizontal plane wave



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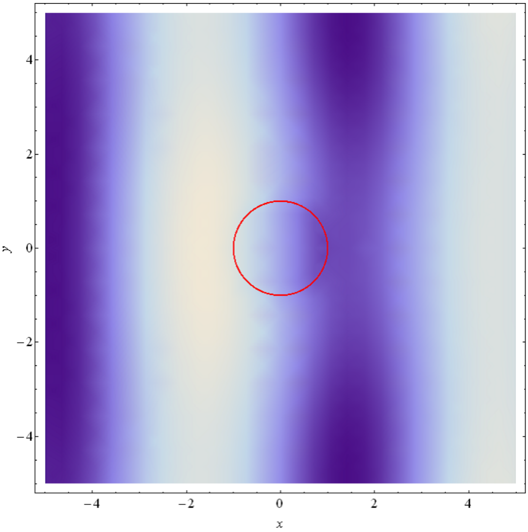
Time propagation of the horizontal plane wave



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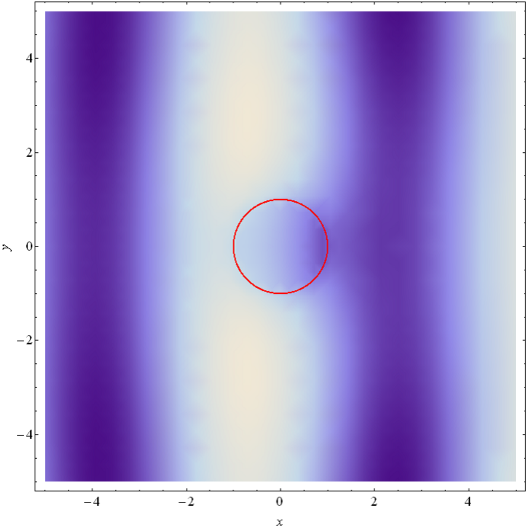
Time propagation of the horizontal plane wave



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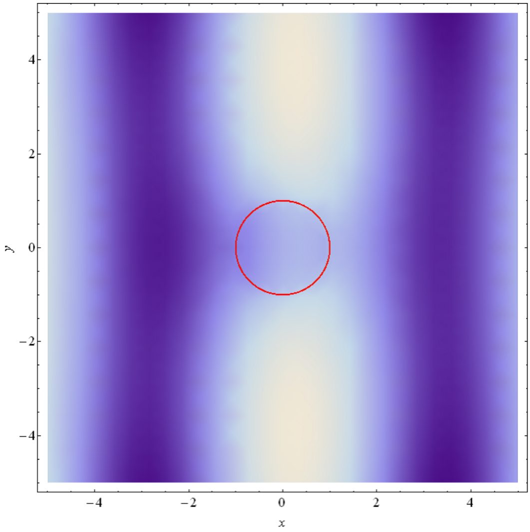
Time propagation of the horizontal plane wave



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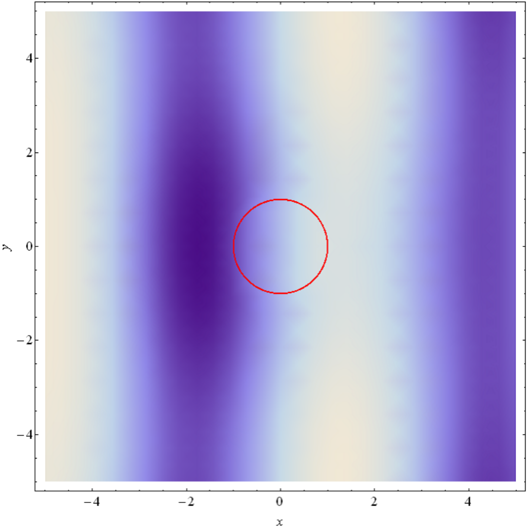
Time propagation of the horizontal plane wave



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Time propagation of the horizontal plane wave

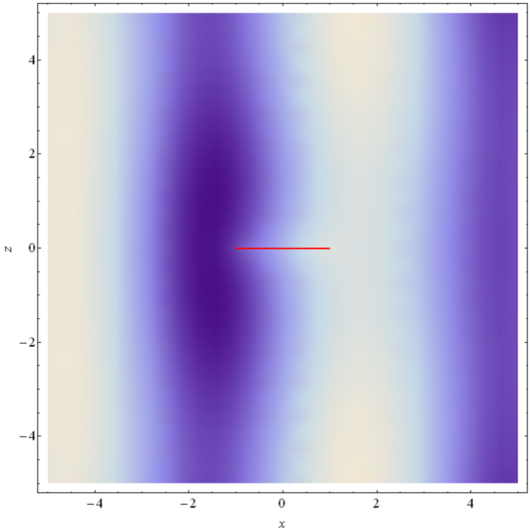
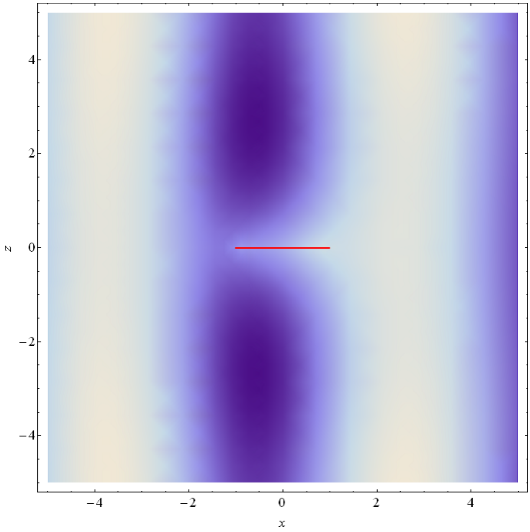


Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the horizontal plane wave



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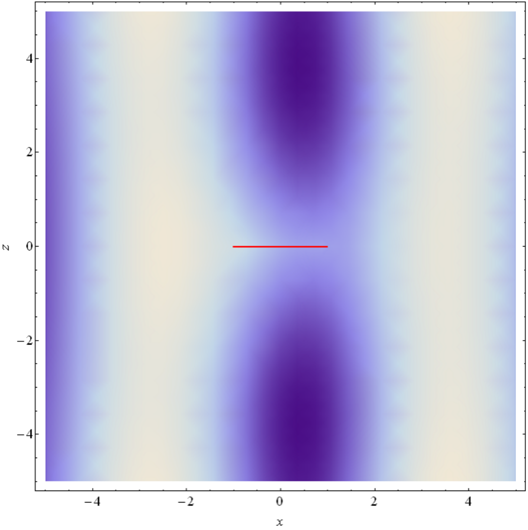

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Time propagation of the horizontal plane wave

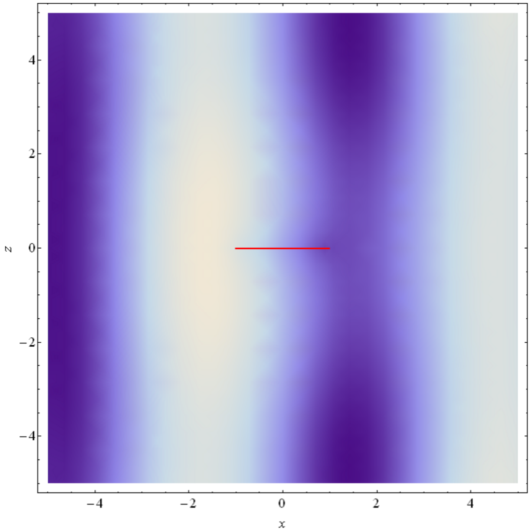


Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the horizontal plane wave

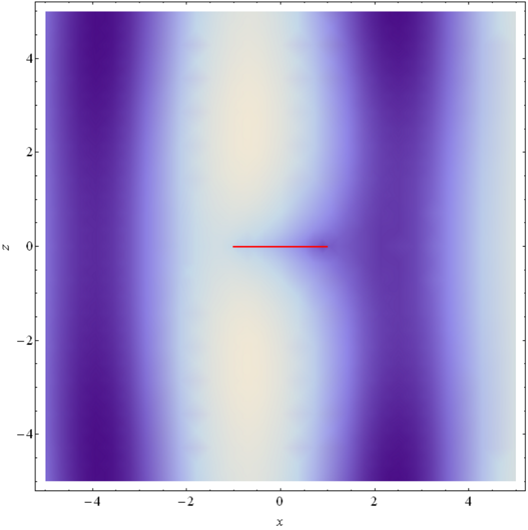


Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the horizontal plane wave

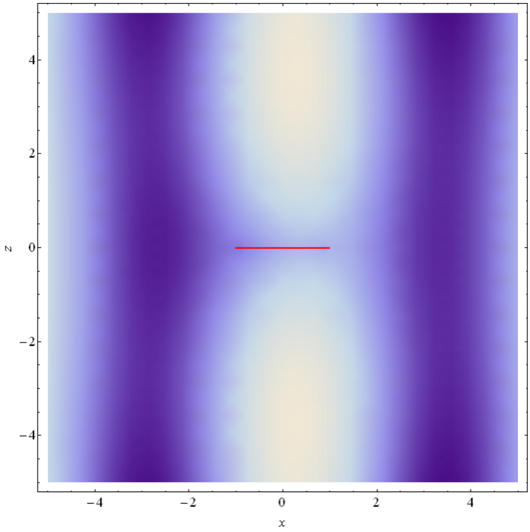


Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the horizontal plane wave

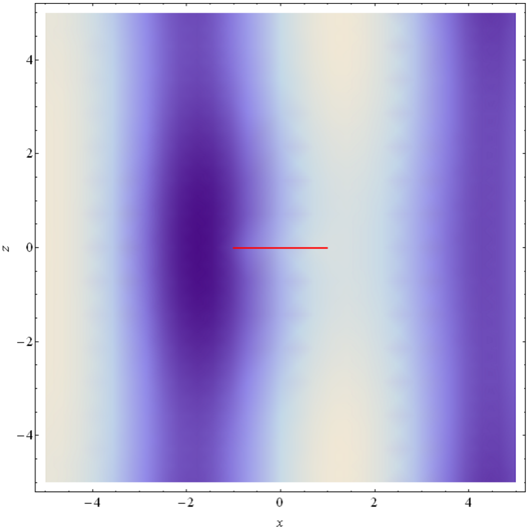


Figure: The imaginary part of the incident plane wave on xz-plane.

Numerical calculation of the scattering wave

Next we assume $a = 1$ and the incident direction is x_3-direction ($p = (0,0,1)$), so $k = 1$, $\tau = 0$, $\psi = 0$. The approximation of the incident plane wave is

$$W_- e^{ix_3} \sim e^{ix_3} + c^2_{0,0}\left(e^{i\delta^0_{0,1}} R^{(5)}_{00} - R^{(1)}_{00}\right)(-i, i\sinh\xi) \cdot S_{00}(-i,\cos\eta) S_{00}(-i,1).$$

From the next page, we shall again exhibit the time propagation of the incident plane wave, by plotting the imaginary part of the wave function on xy-plane and xz-plane.

Time propagation of the vertical plane wave

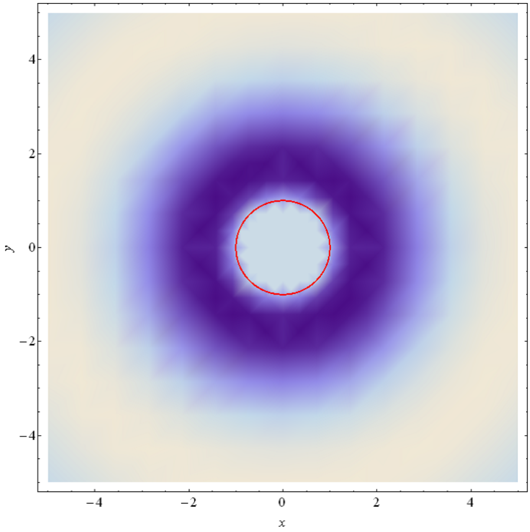


Figure: The imaginary part of the incident plane wave on xy-plane.

Time propagation of the vertical plane wave

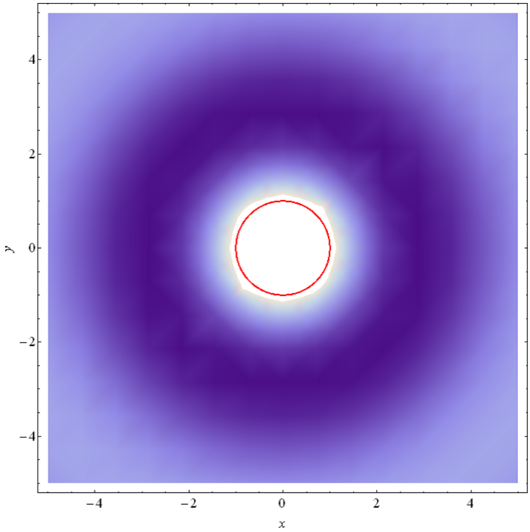


Figure: The imaginary part of the incident plane wave on xy-plane.

Time propagation of the vertical plane wave

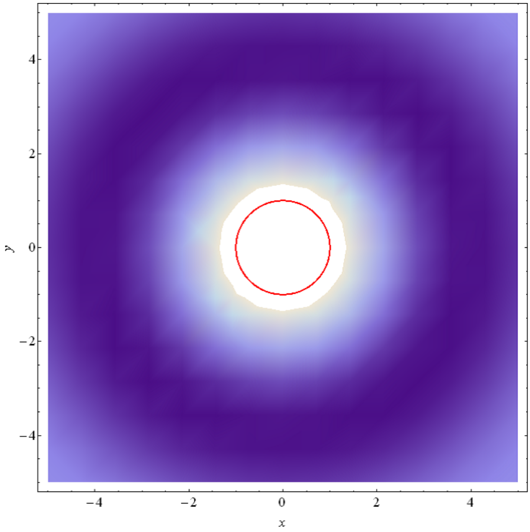


Figure: The imaginary part of the incident plane wave on xy-plane.

Time propagation of the vertical plane wave

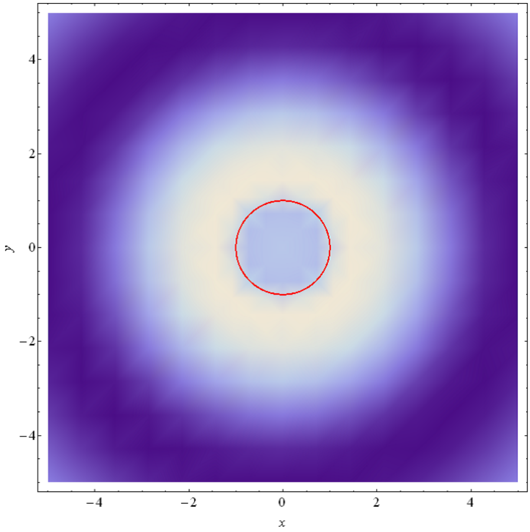
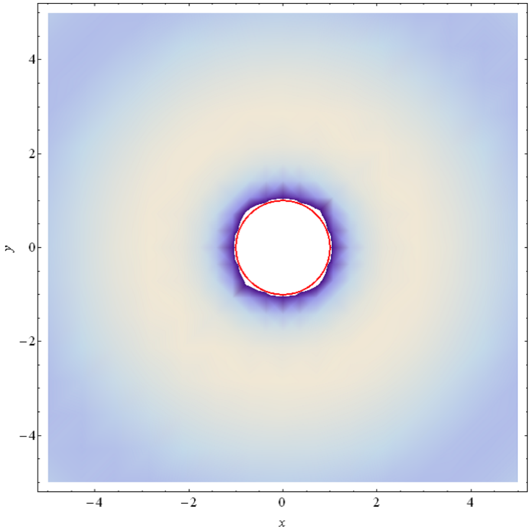


Figure: The imaginary part of the incident plane wave on xy-plane.

Time propagation of the vertical plane wave



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Time propagation of the vertical plane wave

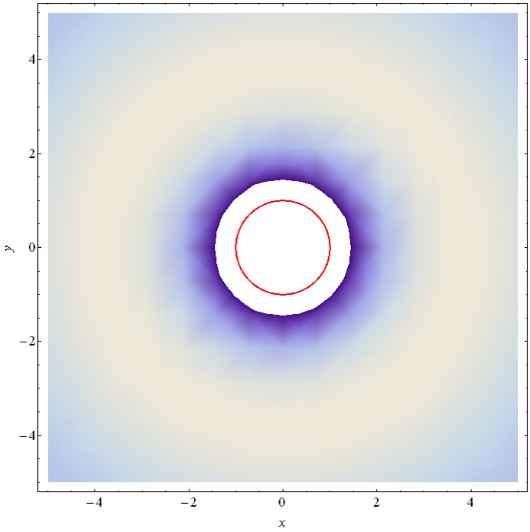

Figure: The imaginary part of the incident plane wave on xy-plane.

Time propagation of the vertical plane wave

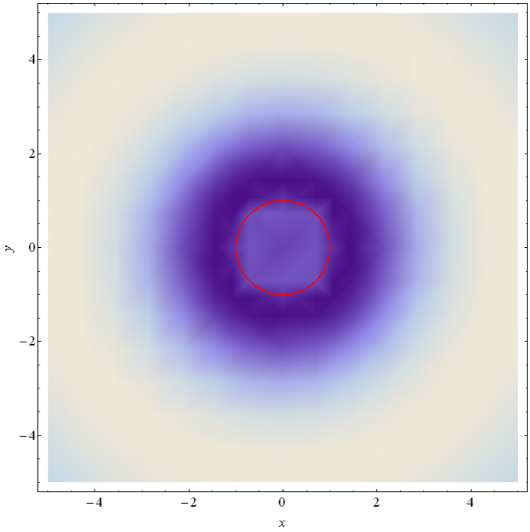

Figure: The imaginary part of the incident plane wave on xy-plane.

Time propagation of the vertical plane wave

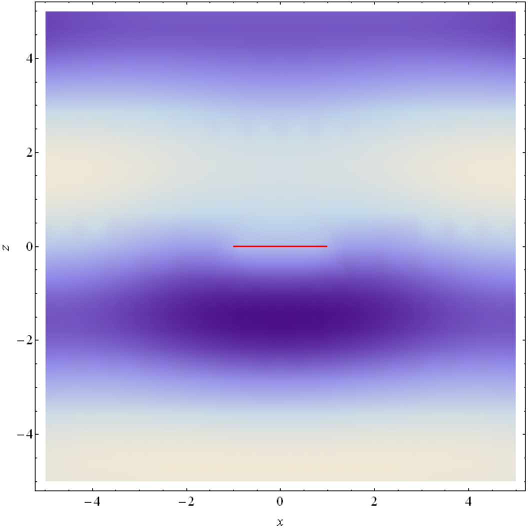

Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the vertical plane wave

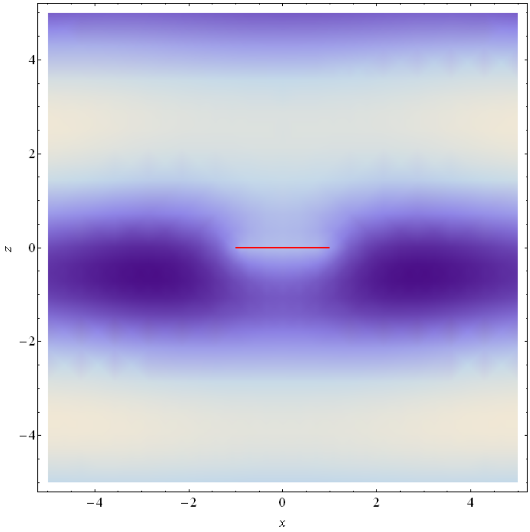

Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the vertical plane wave

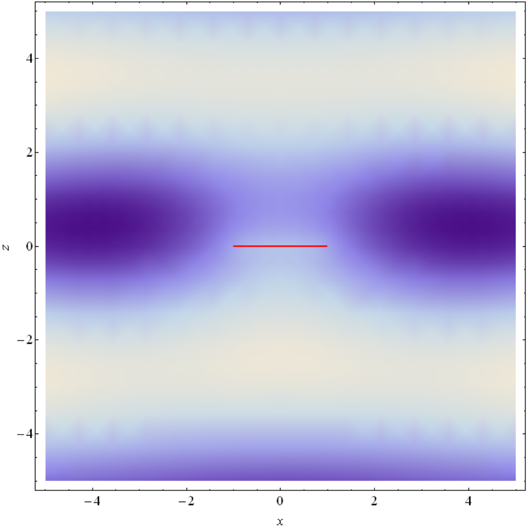

Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the vertical plane wave

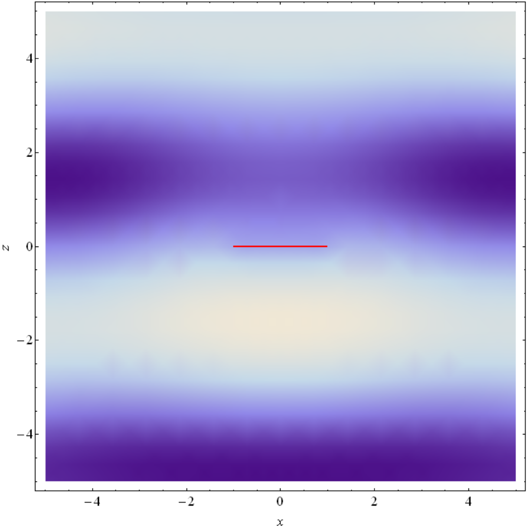

Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the vertical plane wave

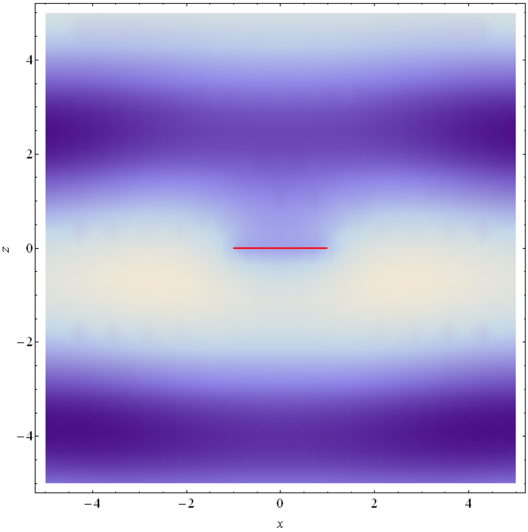

Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the vertical plane wave

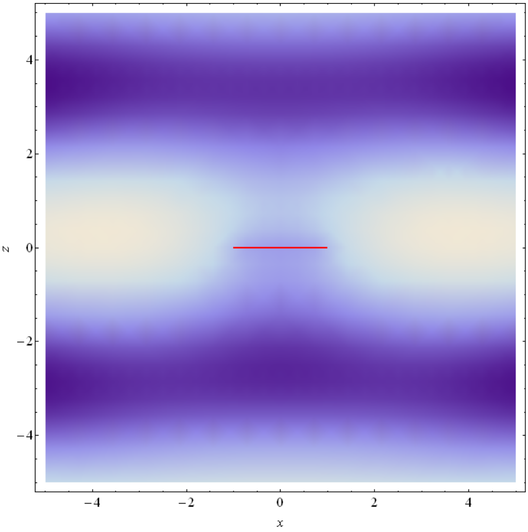

Figure: The imaginary part of the incident plane wave on xz-plane.

Time propagation of the vertical plane wave

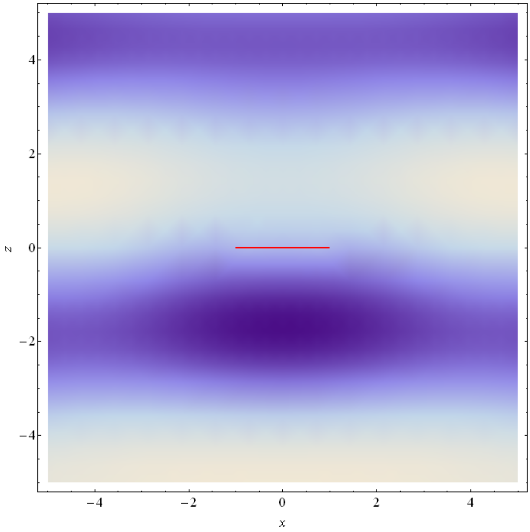

Figure: The imaginary part of the incident plane wave on xz-plane.

Remaining problems

(1) What we exhibited here are the imaginary part of the wave functions, not the interference pattern in the real experiment. How should we take the physical parameters?

(2) We need more technique for the numerical calculation. Sometimes results by Mathematica are unreliable...

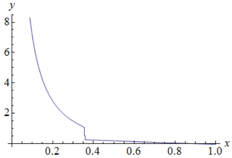

Figure: The graph of $(R_{11}^{(2)})'(-i, ix)$ by Mathematica?

Formulas in Flammer's book might help us.