The Level Set Method and Schrödinger's Equation

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Outline

- Original level set method
  (Osher and Sethian)

- Level set method for higher codimensional objects
  (Joint with Burchard, Merriman, Osher)

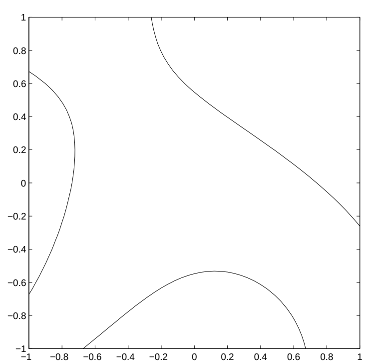
- Isotropic and anisotropic geometrical optics
  (Joint with Kang, Osher, Qian, Shim, Tsai)

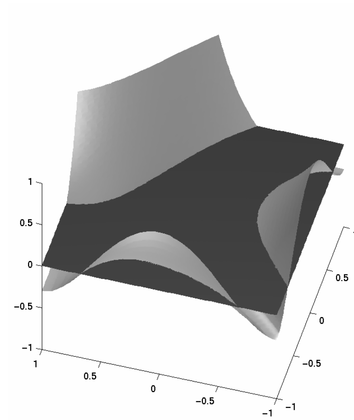
- Wavefronts and Schrödinger's equation
  (Joint with Liu, Osher)

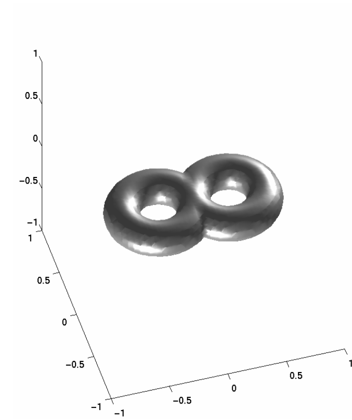
The Original Level Set Method

Framework involves representing objects implicitly as the zero level set of a function, the level set function.

Operate on function instead of object. Numerically, in the ambient space (on uniform grid) instead of parametrized representation.







Evolution and Reconstruction

To move objects, move level set function ϕ instead, usually under a PDE of the form

$$\phi_t + v \cdot \nabla \phi = 0,$$

where v is a given or calculated velocity field.

v can be of the form $v(x, t)$, or can depend on ϕ and its derivatives (curvature flow, Osher and Sethian), or can be linked with other quantities and equations (solidification, Chen, Merriman, Osher, Smereka).

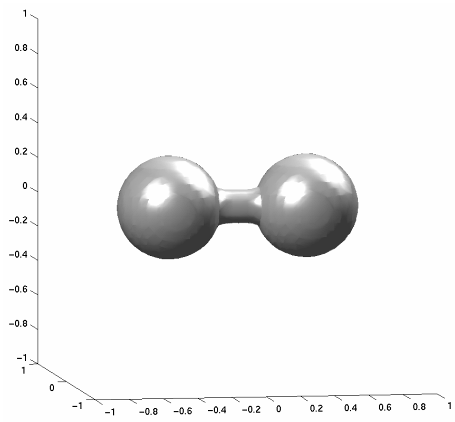
Finally, can recover desired object through interpolation on a grid over the ambient space.

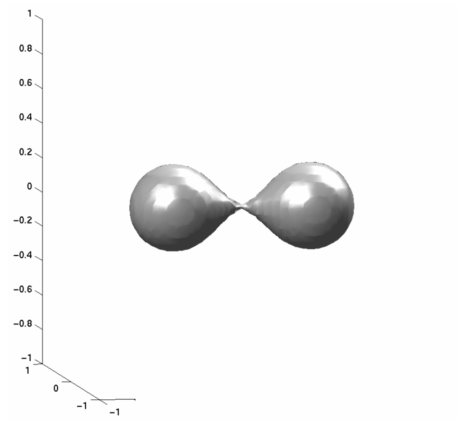
Advantages

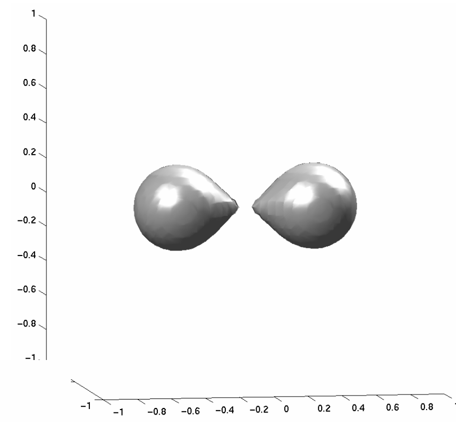
- Easy numerics and automatic resolution (from uniform grid).
- Automatic topological changes (seen in two phase flow, segmentation,. . .).
- Links with geometry, PDE's, and variational formulations.

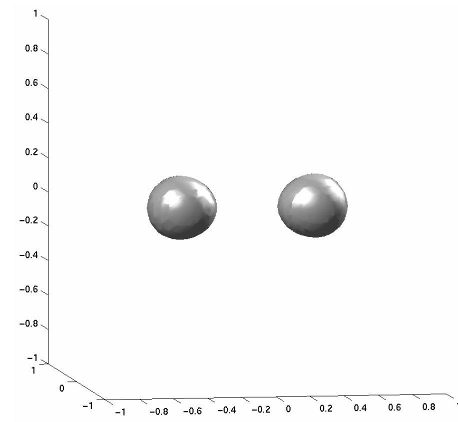
Thus level set methods can be found in many applications such as image processing, materials science, optimal control,. . . (see Osher and Fedkiw)

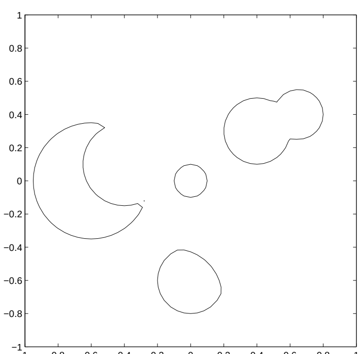
Applications

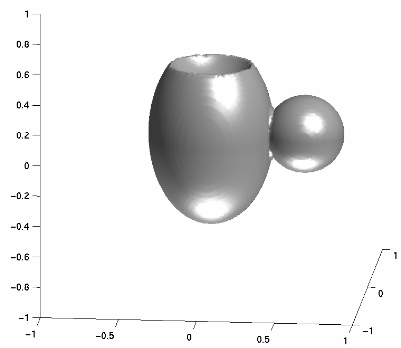


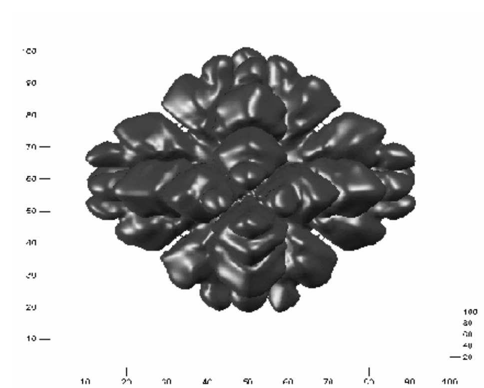












Fix of Disadvantages

Most noticeable disadvantage is in efficiency. Now working one dimension higher.

Fix for this is local level set method (Adalsteinsson and Sethian, Peng, Merriman, Osher, Zhao, Kang)

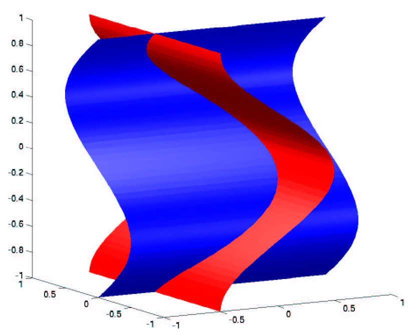
Idea is work only at points in a small neighborhood of object of interest. Size of neighborhood related to spatial step size. Tools to remove the effects of the neighborhood boundaries.

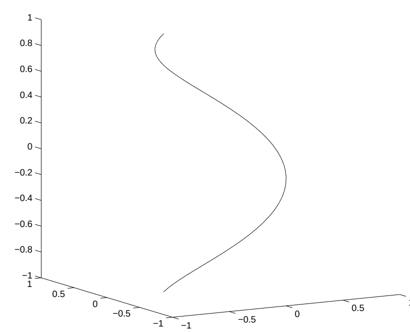
Net effect is retention of efficiency at cost of programming (especially for savings in memory).

Higher Codimensional Objects

The representation, however, does not work well on higher codimensional objects. The problems are in unstable, inaccurate representation and loss of topological changes (Ambrosio and Soner).

The vector valued level set function bypasses these difficulties. Now represent object as the zeros of a vector valued function.





Evolution

Evolve components of vector valued level set function to evolve object.

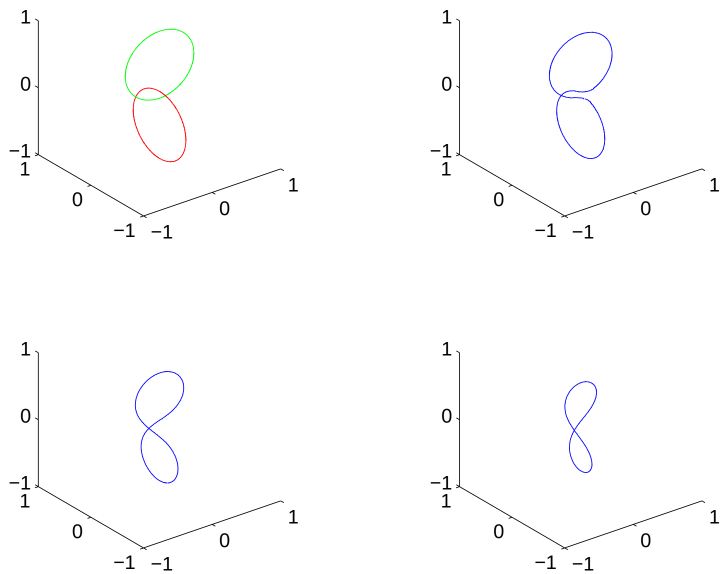
If v is globally defined velocity field, then

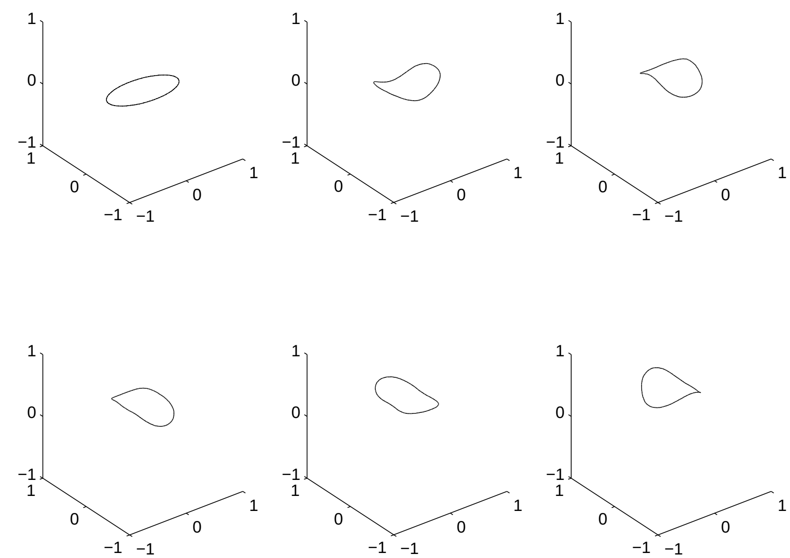
$$(\phi_j)_t + v \cdot \nabla \phi_j = 0,$$

gives desired evolution of object under v, where ϕ_j are the components of the level set function.

v can be a general quantity as discussed before.

Advantages





Efficiency

If ambient space is n dimensional and object of interest is k dimensional, then use an $n-k$ component level set function.

Now working globally in n dimensional space becomes very inefficient.

But local level set ideas still apply and have been implemented (neighborhood, reduction of boundary effects).

Main difficulty once again in programming.

Applications

- Geometric motions (curvature and binormal flows)

- Motions of curves constrained on surfaces (joint with Burchard, Merriman, Osher)

- Dislocations (joint with Xiang, Srolovitz, E)

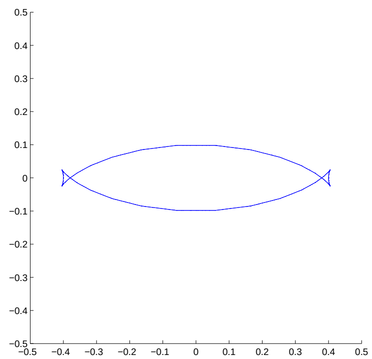
- Isotropic and anisotropic geometrical optics

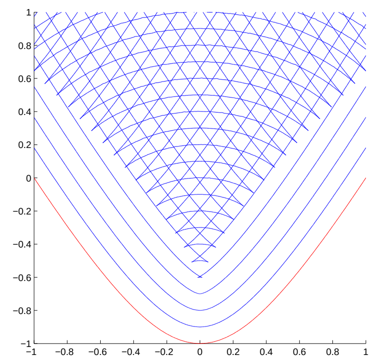
We now visit the framework we use for Schrödinger's equation.

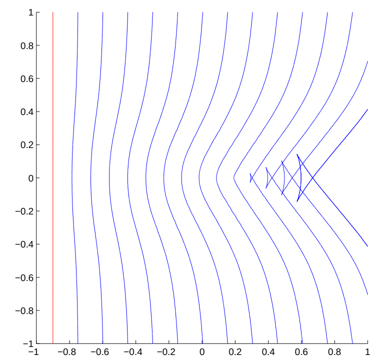
Geometrical Optics

Another difficulty for level set methods is in not enforcing topological changes.

This occurs in geometrical optics, where wavefronts pass through themselves and each other (multivaluedness).







Details

Geometrical optics comes from an approximation for high frequency wave propagation. Here the wave equation reduces to the (time dependent) eikonal equation. (Anisotropic wave and eikonal equations in anisotropic case)

There are applications, for example, in seismic data processing, in Kirchoff migration, tomography velocity analysis, and inversion, for oil industry applications.

Our interest is in generation of wavefronts (points of constant traveltime from given sources in the given medium), which are derived from the eikonal equation.

Viscosity Solutions

Eikonal equation (isotropic case)

$$\phi_t + c|\nabla\phi| = 0,$$

where c is the local wave speed.

Zeros of ϕ at time t attempts to give the wavefronts of traveltime t.

Benefits are in Eulerian framework (automatic resolution). Except the viscosity solution is not the desired solution.

Much work has been devoted to fixing this.

Ray Tracing

Another way to interpret wavefront evolution is through ray tracing.

Wavefronts follow the Hamiltonian system of ODE's agreeing with the characteristics of the eikonal equation.

Ray tracing allows for multivalued solutions. But they lead to Lagrangian methods where numerical resolution becomes a problem, especially for diverging wavefronts.

Work by Vinje and collaborators have been devoted to fixing this.

Phase Space

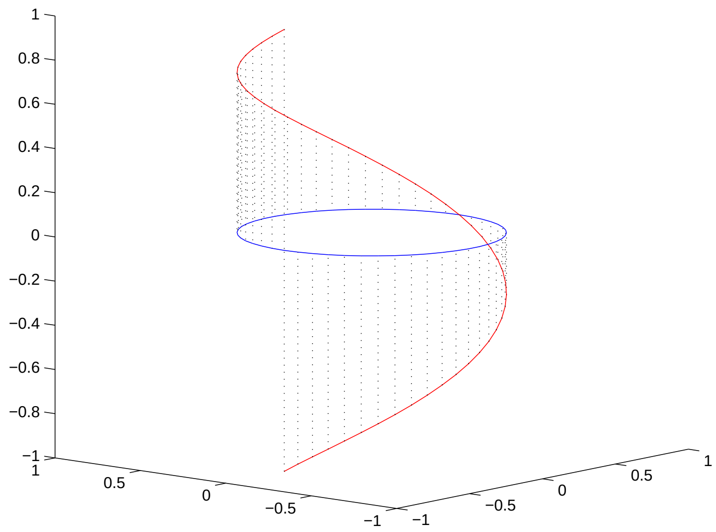
We may, however, consider another space in which to view wavefronts and their evolution.

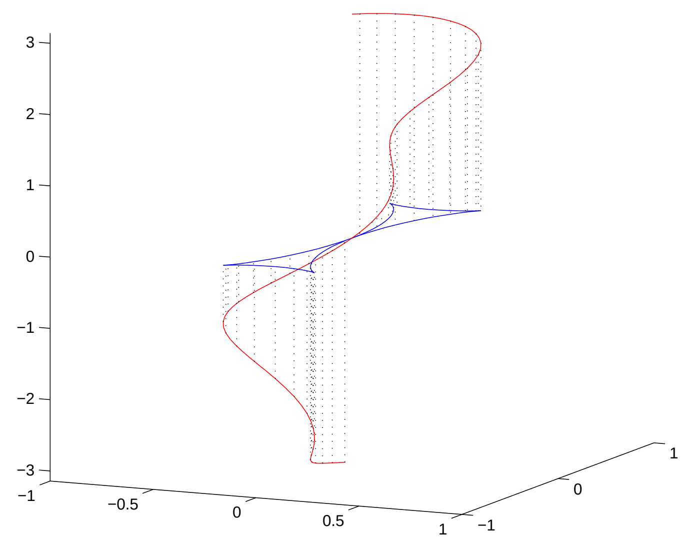
Phase space at a given time is composed of (x, p), where x is spatial location and p is local phase direction.

In this setting, wavefronts are represented by bicharacteristic strips, which form $n-1$ dimensional Lagrangian submanifolds, that evolve under the Liouville equation.

Study of this is well known in the theoretical aspect (see, e.g., Arnol'd).

Phase Space Objects





Numerical Advantages

Engquist, Runborg, Tornberg first realized the advantages of numerical calculations set in phase space for this problem.

Advantages:

- Phase space handles multivalued wavefronts through smooth bicharacteristic strips.
- Using an Eulerian framework in conjunction with the Liouville PDE in phase space handles resolution.

Engquist, Runborg, Tornberg used the segment projection method for their Eulerian framework. Here we use a level set approach.

Level Set Approach

Notice bicharacteristic strips are objects of high codimension in phase space. Thus in a level set approach, a vector valued level set function ϕ is needed to represent these objects.

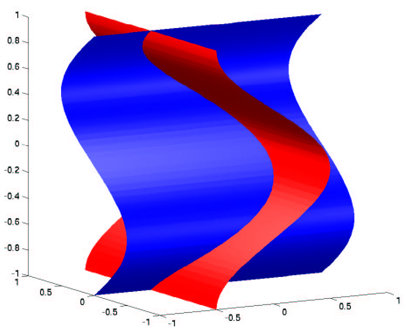
Evolution of the level set functions is according to the Liouville PDE which is a transport equation:

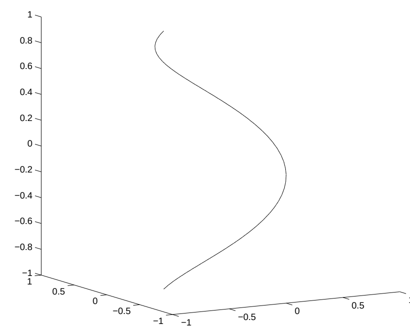
$$(\phi_j)_t + v(x,p) \cdot \nabla_{x,p} \phi_j = 0,$$

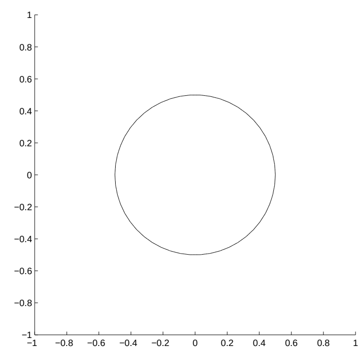
where $v(x,p)$ consists of the characteristics of the eikonal equation.

Solve to desired time and plot the zero level set.

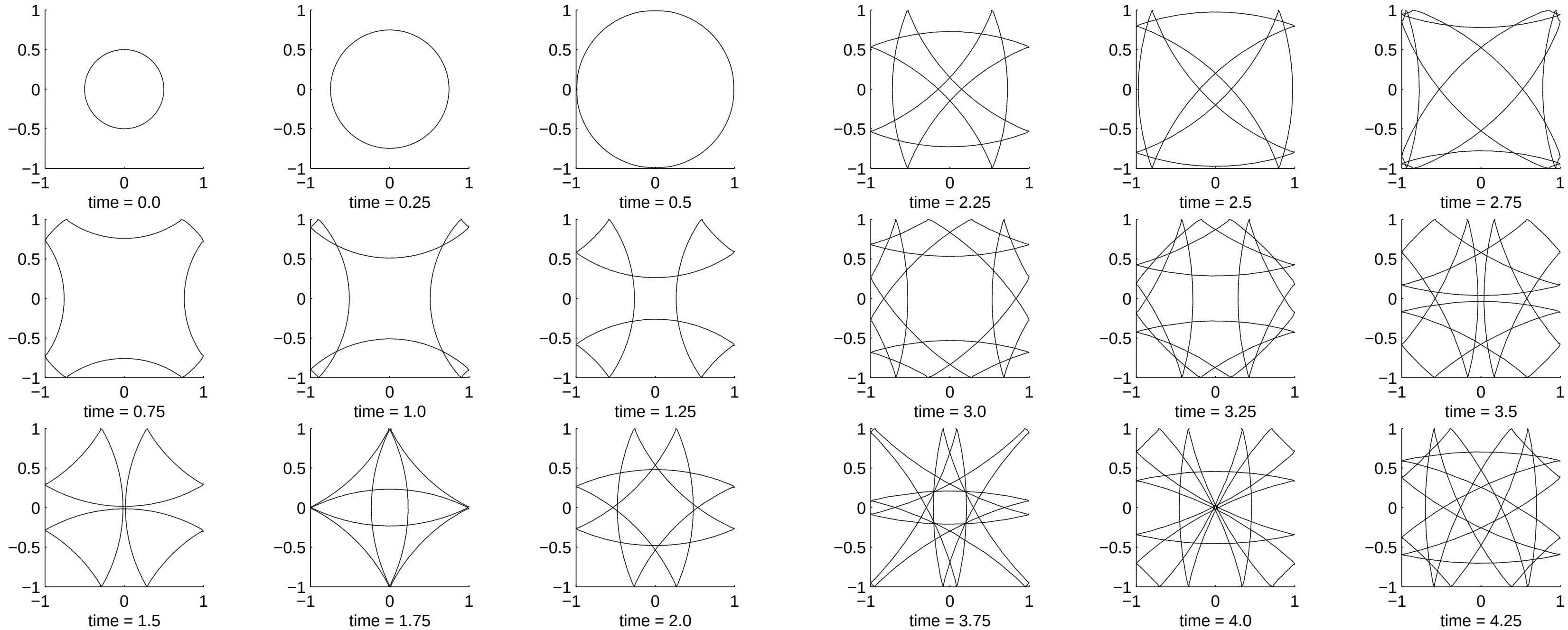
Level Set Framework







Reflection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time = 0.5
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time = 2.5
time = 2.75
time = 0.75
time = 1.0
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time = 3.0
time = 3.25
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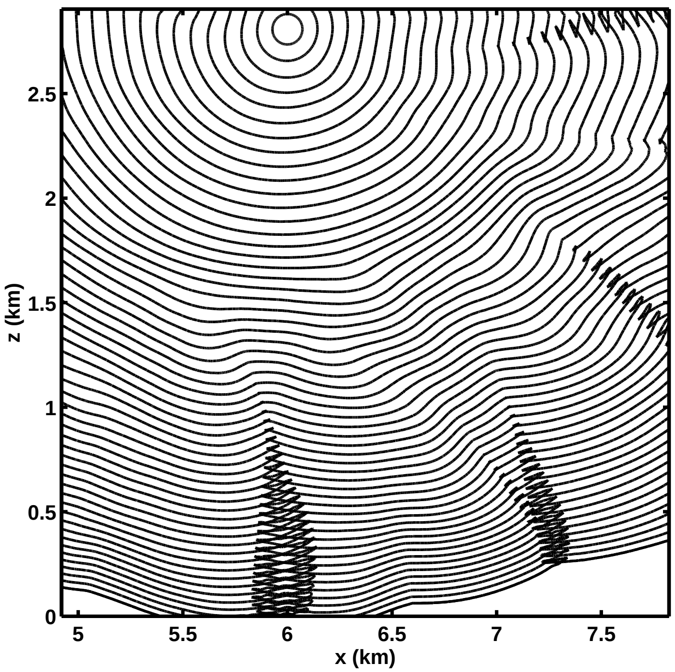
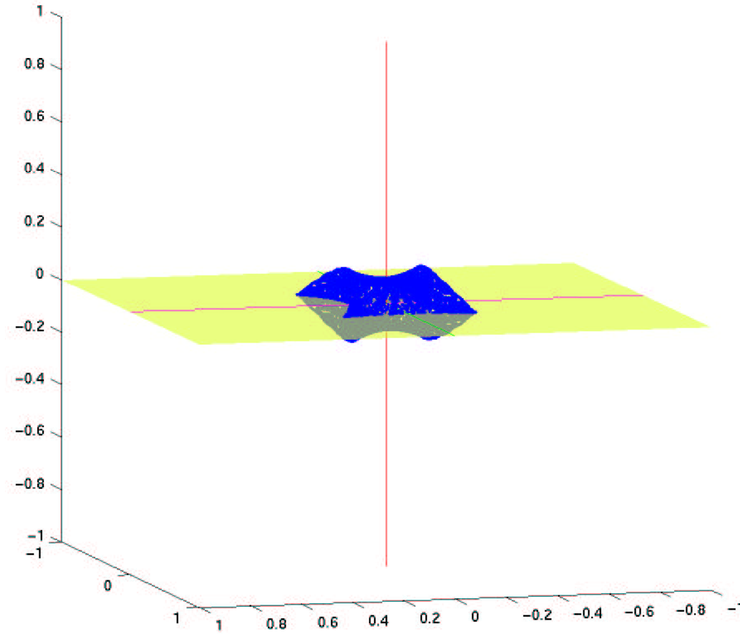
time = 1.5
time = 1.75
time = 2.0
time = 3.75
time = 4.0
time = 4.25

Anisotropic and 3D





Linear Schrödinger Equation

We can look at something similar for Schrödinger's equation.

We consider the linear Schrödinger equation with $x \in \mathbf{R}^n$,

$$i\epsilon\partial_t\psi = -\frac{\epsilon^2}{2}\Delta\psi + V(x)\psi,$$

with high frequency initial data

$$\psi(x,0) = A_0(x)e^{i\frac{S_0(x)}{\epsilon}}.$$

ψ is the wave function.
$V(x)$ is a given potential function.
$\epsilon > 0$ is a re-scaled Planck constant.

Phase and Amplitude

In the semi-classical regime where ϵ is small, make the ansatz

$$\psi^\epsilon = A^\epsilon e^{i\frac{S}{\epsilon}},$$

with

$$A^\epsilon = A + \epsilon A_1 + \epsilon^2 A_2 + \dots.$$

S is the phase.
A^ϵ is the amplitude, with A its leading order term.

Plug this ansatz in and match terms with respect to ϵ to arrive at PDE's for the phase and the amplitude.

Hamilton-Jacobi Equation

In the lowest order, the phase S satisfies a nonlinear first order Hamilton-Jacobi equation

$$\partial_t S + H(x, \nabla_x S) = 0,$$

where

$$H(x,p) = \frac{|p|^2}{2} + V(x).$$

Furthermore, amplitude up to leading order satisfies the PDE,

$$\partial_t A^2 + \nabla \cdot (A^2 \nabla S) = 0.$$

We may consider wavefronts again using this Hamilton-Jacobi equation.

Characteristics

Solution S of the Hamilton-Jacobi equation can be obtained locally by the method of characteristics.

Set $p = \nabla_x S(x,t)$.

Starting with a hypersurface, the initial wavefront, where the initial phase is constant, propagate points under the ODE's

$$\begin{aligned} \frac{dx}{dt} &= \nabla_p H(x,p), \\ \frac{dp}{dt} &= -\nabla_x H(x,p) \end{aligned}$$

The phase S also propagates under the ODE

$$\frac{dS}{dt} = p \cdot \nabla_p H(x,p) - H(x,p).$$

Multivalued Solutions

However, as in geometrical optics, rays may intersect causing multivalued solutions. This means viscosity solutions of the Hamilton-Jacobi equation are not desired.

Thus numerical schemes for constructing wavefronts for the Schrödinger equation will encounter the same difficulties as those tackling the geometrical optics problem.

Now we can use the techniques mentioned previously to overcome the difficulties: Eulerian framework and phase space calculations.

In Phase Space

In $2n$ dimensional phase space (for n dimensional spatial space), the $n-1$ dimensional bicharacteristic strips evolve according to the Liouville equation using characteristic directions

$$v(x,p) = \begin{pmatrix} \nabla_p H(x,p) \\ -\nabla_x H(x,p) \end{pmatrix}.$$

The phase similarly follows these directions, though its value changes according to the forcing term $p \cdot \nabla_p H(x,p) - H(x,p)$.

Level Set Framework

We represent bicharacteristic strips using the level set method. Use a $n+1$ component vector valued level set function ϕ.

Evolution of ϕ in phase space is according to Liouville equation on components,

$$(\phi_j)_t + v \cdot \nabla_{x,p} \phi_j = 0$$

or, written out,

$$(\phi_j)_t + \nabla_p H(x,p) \cdot \nabla_x \phi_j - \nabla_x H(x,p) \cdot \nabla_p \phi_j = 0.$$

Similarly, evolution of S is under the equation

$$S_t + \nabla_p H(x,p) \cdot \nabla_x S - \nabla_x H(x,p) \cdot \nabla_p S = p \cdot \nabla_p H(x,p) - H(x,p).$$

Differences With Previous

The procedure taken is analogous to the previous one for geometrical optics. One major difference, however, is that p cannot be simplified to θ, which denotes the angle of p.

For example, for

$$H(x,p) = \frac{|p|^2}{2} + \frac{|x|^2}{2},$$

$|p|$ may become zero on bicharacteristic strips.

Thus, we work in full $2n$ dimensional phase space (4D for 2D spatial space and 6D for 3D spatial space).

Numerical Setting

The level set framework allows for a uniform grid to be placed over phase space. The various PDE's can be discretized using finite difference methods over this grid.

For the location of wavefronts,

- Calculate v at each gridpoint and initialize level set function.

- Solve the transport equation for each component of ϕ using fourth order SSP-RK in time and fifth order WENO in space up to the desired time.

- Determine the zeros of ϕ and project to spatial space.

Constructing the Initial

Suppose $S_0(x) = C$ gives the initial wavefront. Then one of the components of the initial level set function can be taken to be

$$\phi_1 = S_0 - C.$$

The rest can be taken to satisfy $p = \nabla_x S_0$:

$$\phi_{j+1} = p_j - \partial_{x_j} S_0,$$

for $j = 1, \ldots, n$.

Thus the zero level set of ϕ will represent the bicharacteristic strips associated to the initial wavefront.

Numerical Results

We look at the simpler case of $n = 2$. Thus the vector valued level set function has 3 components.

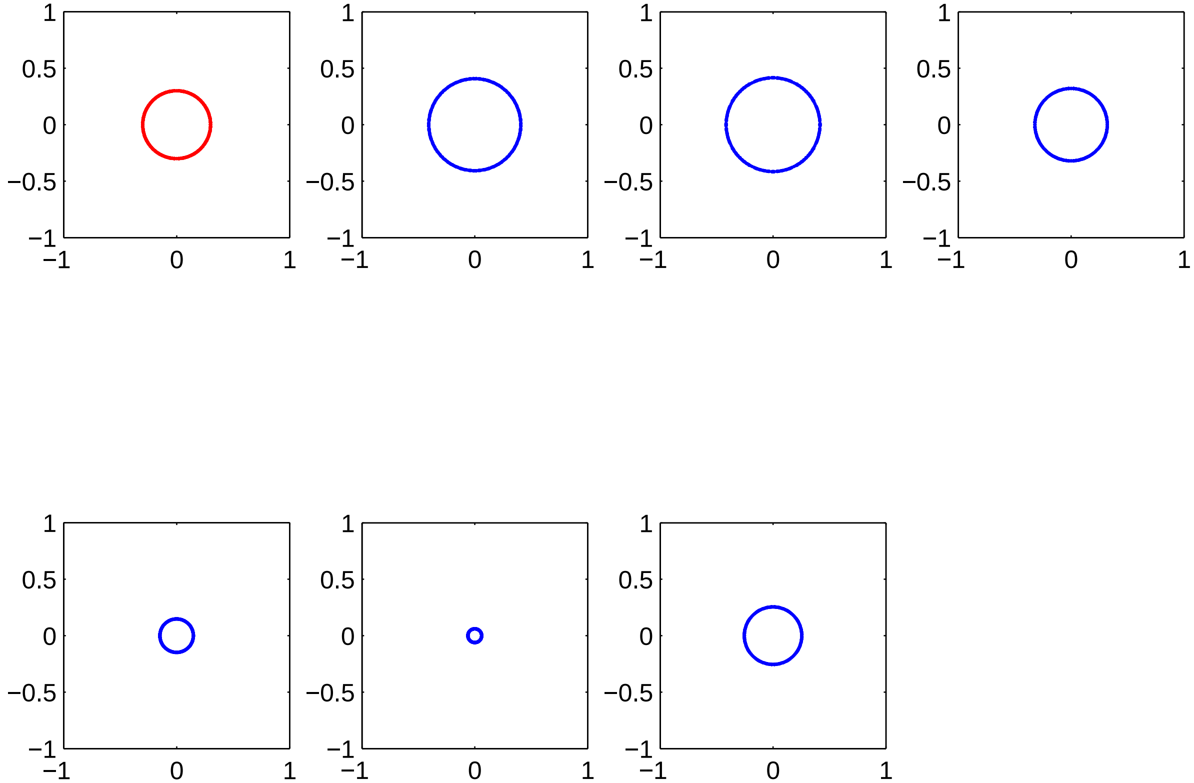
We start with the case of the harmonic oscillator, $V(x) = \frac{|x|^2}{2}$:

$$H(x,p) = \frac{|p|^2}{2} + \frac{|x|^2}{2}.$$

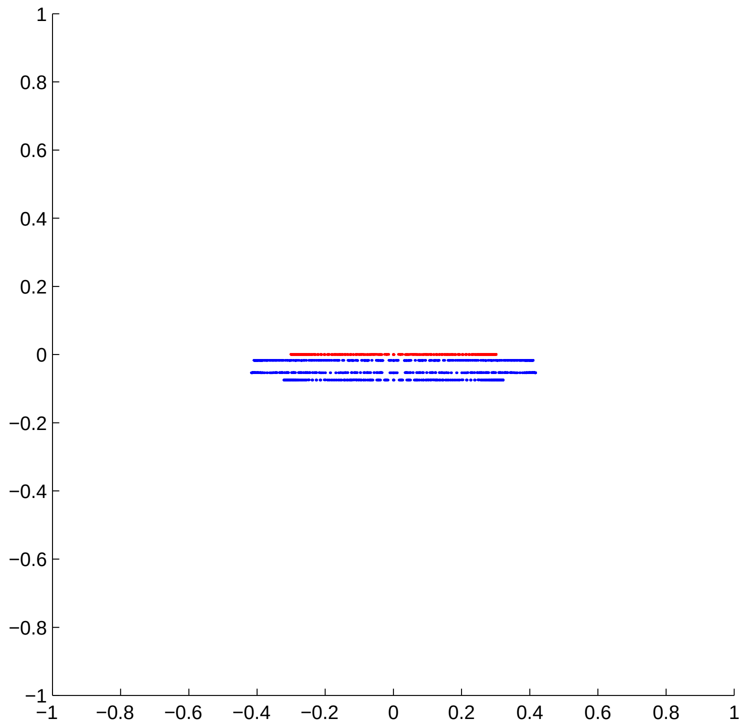
Thus

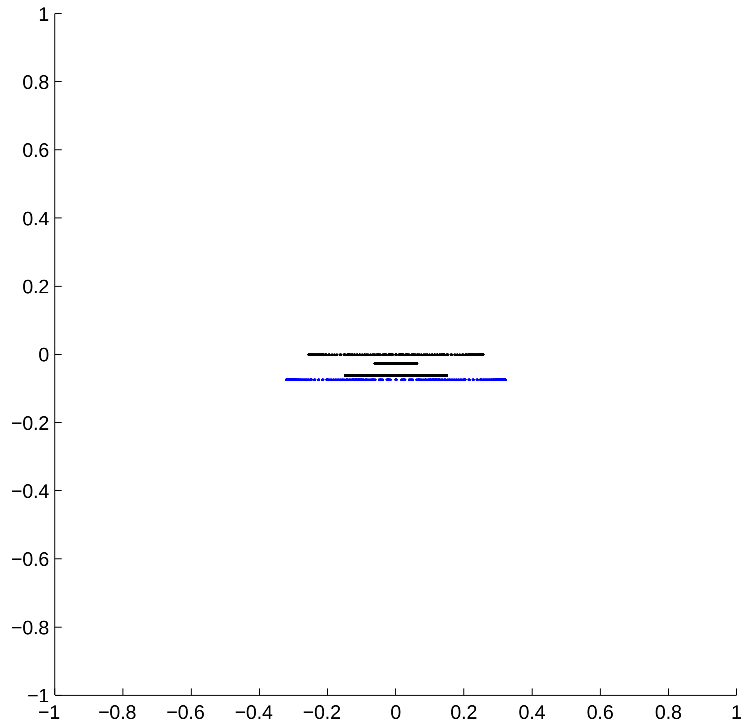
$$v(x_1, x_2, p_1, p_2) = \begin{pmatrix} p_1 \\ p_2 \\ -x_1 \\ -x_2 \end{pmatrix}.$$

We solve the evolution equation for the level set function with different initial wavefronts and initial phase.

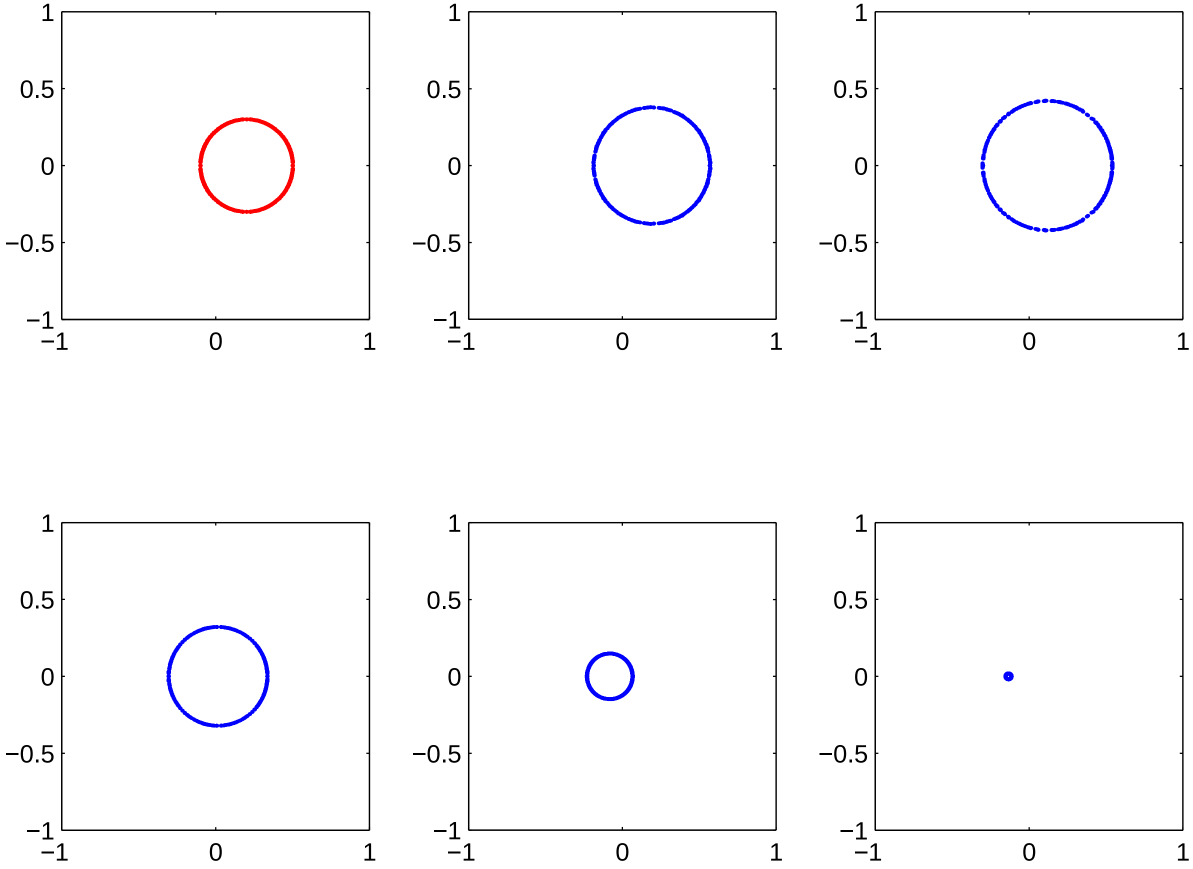


Oscillating Circle

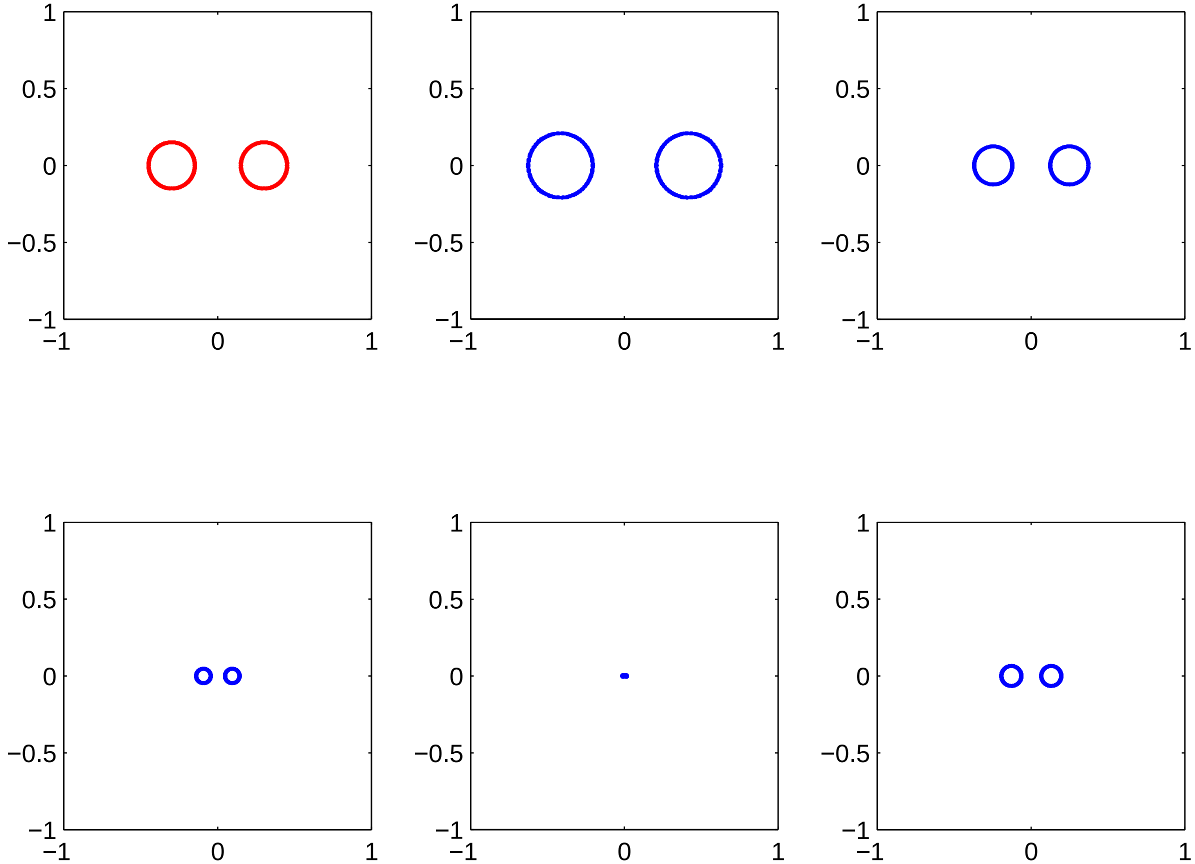




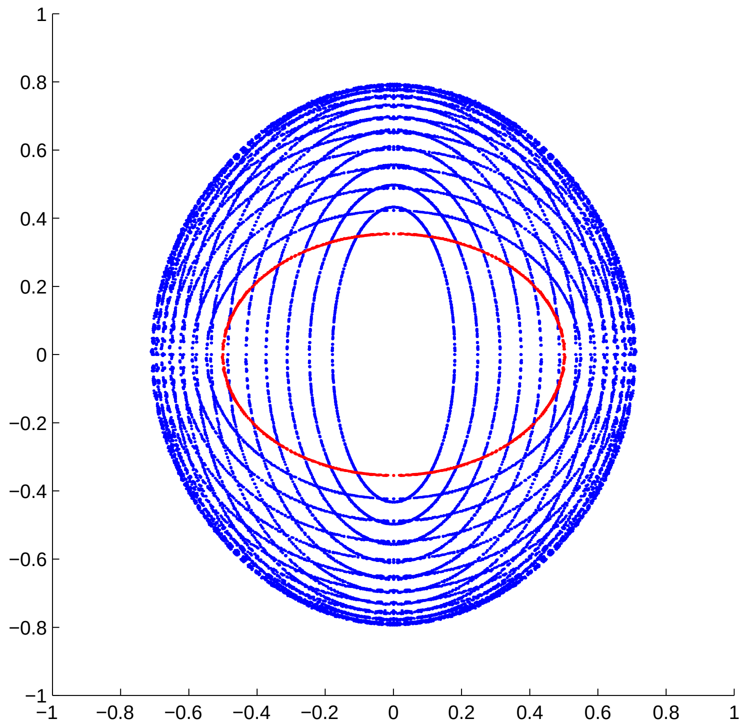
Oscillating Circle Phase

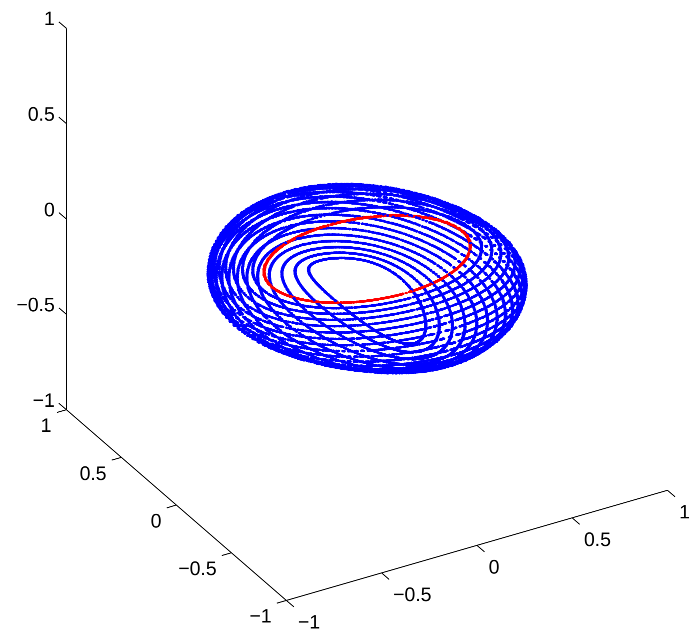


Shifted Circle



Two Circles





Shifted Ellipse Phase

Free Motion

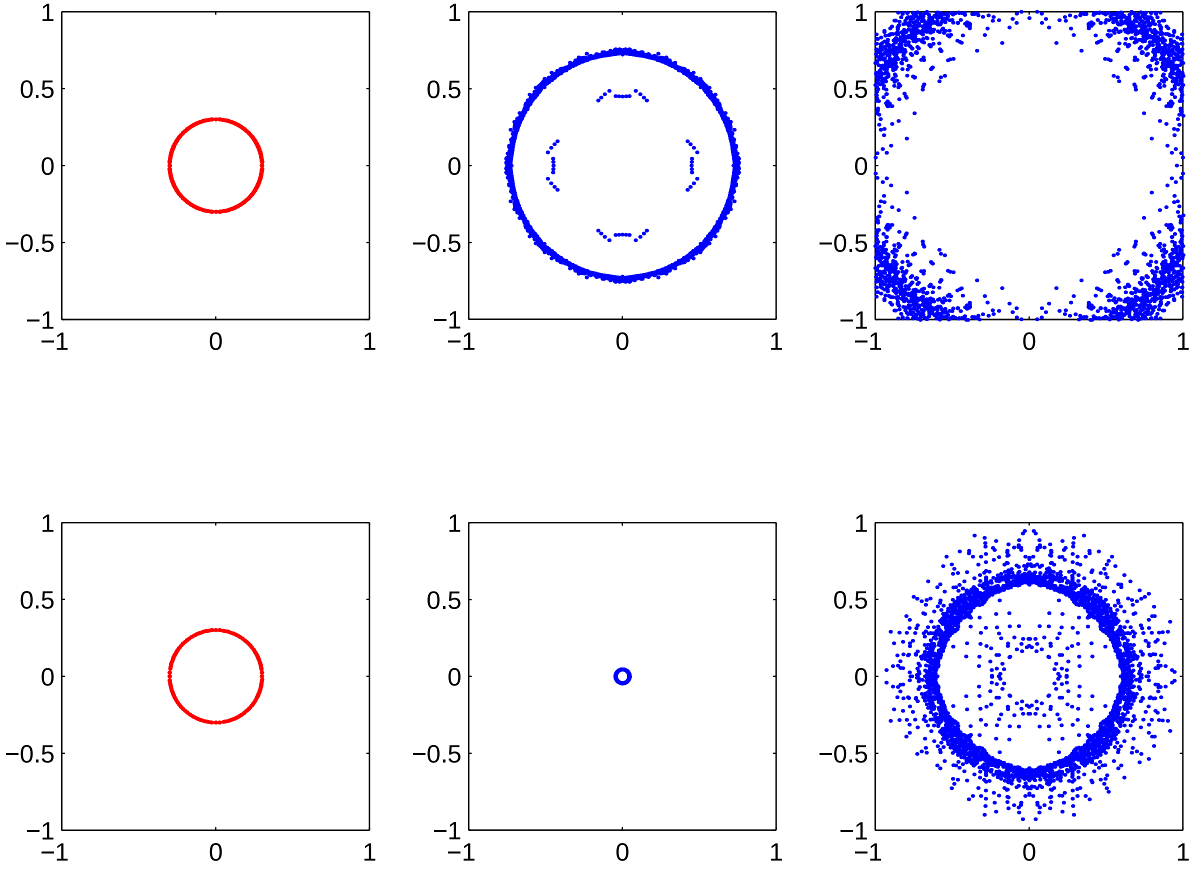
This is the case with $V(x) = 0$,

$$H(x,p) = \frac{|p|^2}{2}.$$

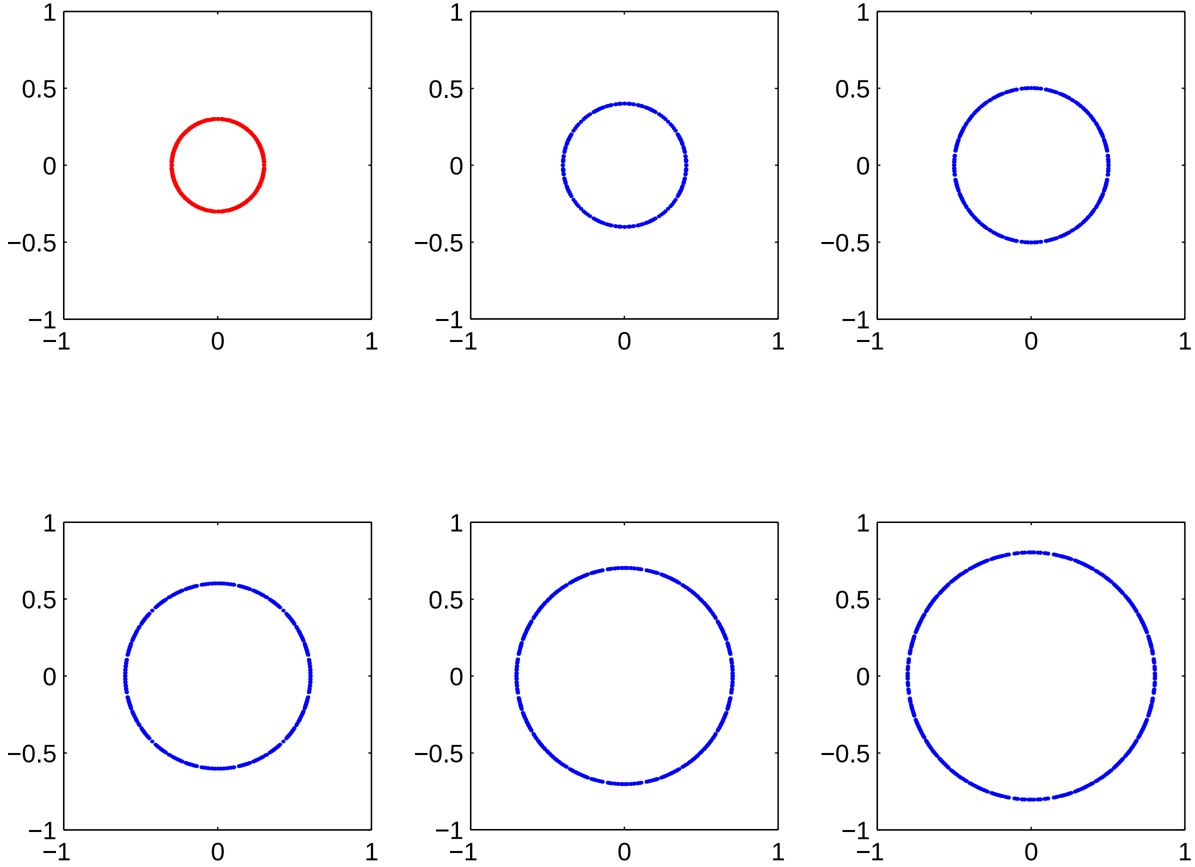
Thus

$$v(x_1, x_2, p_1, p_2) = \begin{pmatrix} p_1 \\ p_2 \\ 0 \\ 0 \end{pmatrix}.$$

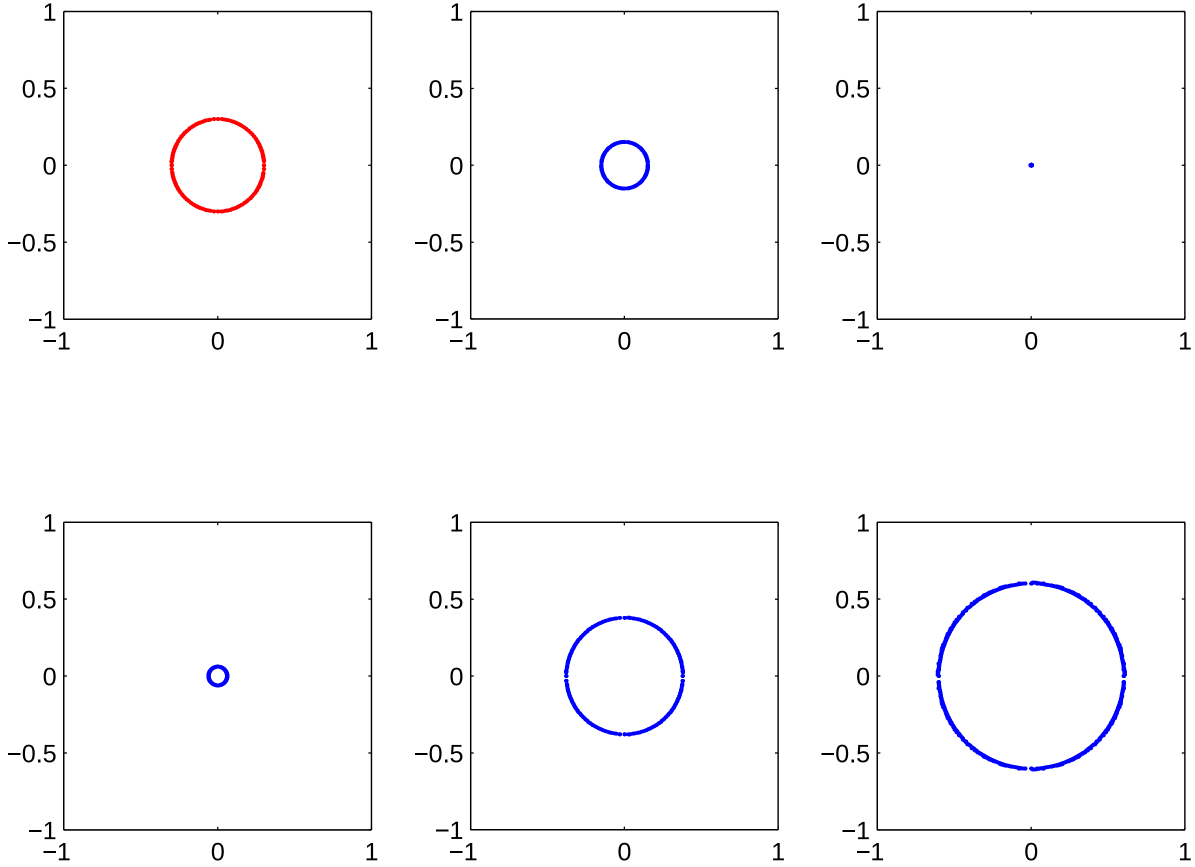
This case can actually be handled in reduced phase space. Furthermore, we see the need for either reinitialization or fine grids.



Bad Effects



Growing Circle



Shrinking Circle

Conclusion

We introduce a numerical algorithm for the construction of wave-fronts in the setting of the linear Schrödinger equation.

This algorithm uses the foundation found in the level set approach for geometrical optics and thus bypasses many difficulties.

Results are satisfactory so far. Of interest is interpretation in the Schrödinger equation setting.