Knotted wave functions

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Prelude

It all began with the simple question:

Are there solutions of the Schrödinger equation
that have the shape of a smoke ring?

The answer exceeded all our expectations

Schrödinger wave equation

$$i\hbar\partial_t\psi(\vec{r},t) = (-\frac{\hbar^2}{2m}\Delta + V(\vec{r}))\psi(\vec{r},t)$$

Hydrodynamic form Erwin Madelung 1926

Hydrodynamic variables: $\psi = R\exp(\frac{i}{\hbar}S)$

Probability density ρ and velocity $\vec{v}$

$$\rho = \psi^*\psi = R^2 \qquad \vec{v} = \frac{\hbar}{2mi}\frac{\psi^*\overleftrightarrow{\nabla}\psi}{\psi^*\psi} = \nabla S$$

Is the probability flow irrotational?

Not if the phase of ψ is singular

Evolution equations for hydrodynamic variables

$$
\begin{aligned}
\partial_t \rho + (\vec{v}\cdot\nabla)\rho &= -\rho\nabla\cdot\vec{v} \\
\partial_t \vec{v} + (\vec{v}\cdot\nabla)\vec{v} &= -\frac{1}{m}\nabla V + \nabla\left(\frac{\hbar^2}{2m^2}\frac{\Delta\rho^{1/2}}{\rho^{1/2}}\right)
\end{aligned}
$$

The vorticity quantization condition must be satisfied for every contour C to make the hydrodynamic formulation equivalent to the original Schrödinger theory

$$
\oint_C d\vec{l}\cdot\vec{v}(\vec{r},t) = \int_S d\vec{n}\cdot(\nabla\times\vec{v}) = \tfrac{2\pi\hbar}{m}\, n
$$

$$
n = 0, \pm 1, \pm 2, \ldots
$$

Vortex lines

Velocity is a gradient $\vec{v} = \nabla S$

Vorticity can be localized only at the singularities of φ

Wave function must be regular

Therefore, ψ must vanish on all vortex lines

Vanishing of ψ gives two equations

$$\mathrm{Re}\psi(\vec{r}, t) = 0$$

$$\mathrm{Im}\psi(\vec{r}, t) = 0$$

Each equation defines a surface in 3D moving in time

The intersection of these two surfaces is a

vortex line moving in time

Orders of magnitude

The characteristic parameter $\hbar/m$ will appear in all formulas

In the case of an electron $\hbar/m$ is of a macroscopic size

$$\frac{\hbar}{m} = 1.16 \cdot \ \mathrm{cm}\frac{\mathrm{cm}}{\mathrm{sec}}$$

At a distance of 1mm from the vortex line the probability flows

around the vortex line about 3 times in a second.

In an atom at a distance of the Bohr radius the probability flows around the vortex line at the speed of $3.5 \cdot 10^5$ meter/sec.

Conservation of vorticity

Vorticity flux trough a surface moving with the fluid is conserved

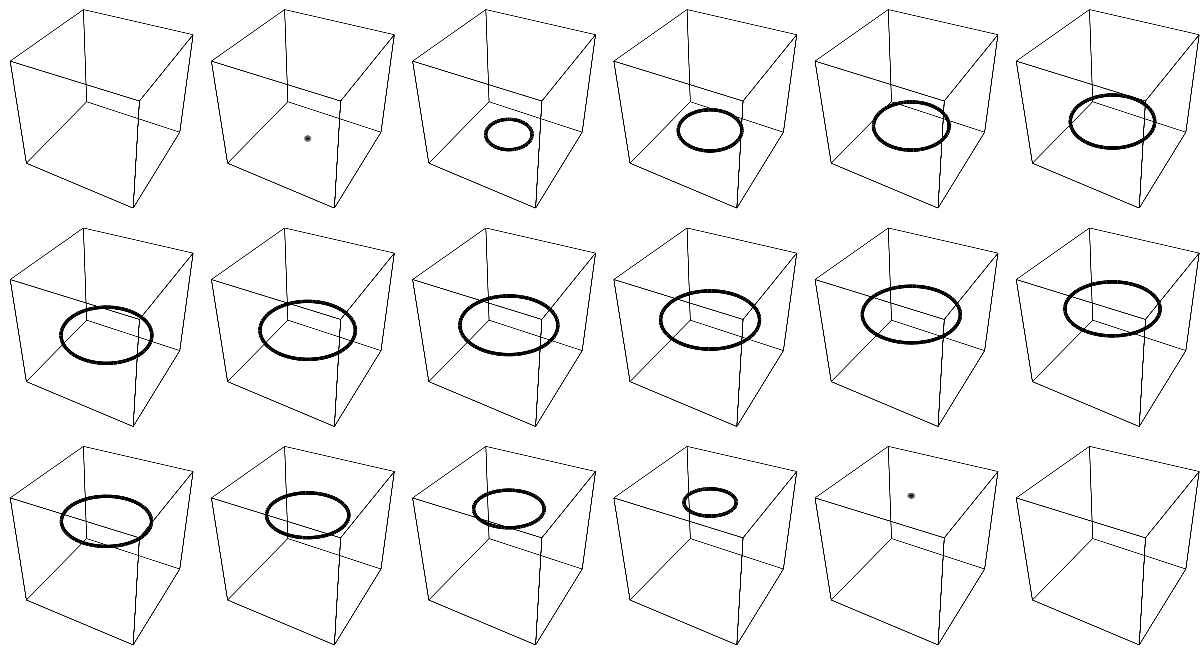
$$\frac{d}{dt}\int_S d\vec{n}\cdot(\nabla\times\vec{v}) = 0$$

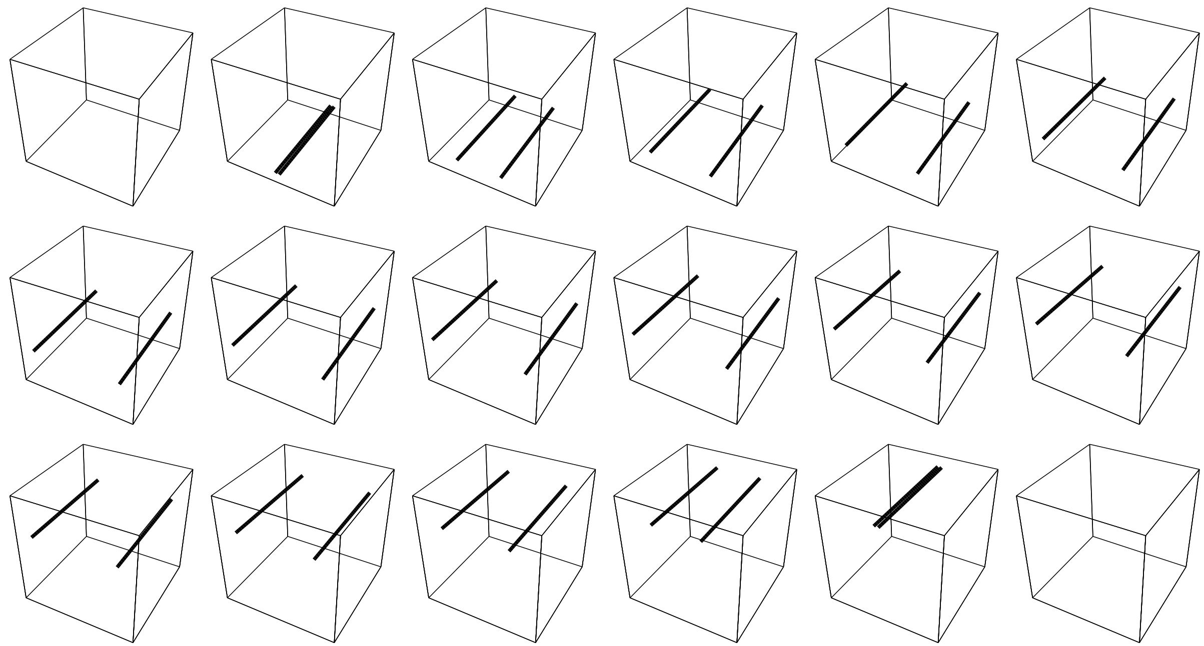
However, it can only change owing to such phenomena as:

a) Vortex lines shrinking to zero or expanding from zero

b) Vortex lines of opposite circulation merging or splitting

These phenomena can be seen in the motion of vortex lines obtained from the Schrödinger equation for a freely moving particle





Manufacturing knotted solutions 1

Take the plane wave:

$$\Psi^P_{\vec{k}}(\vec{r}, t) = \exp\left(i\vec{k} \cdot \vec{r}\right) \exp\left(-\frac{\hbar}{m} \frac{\vec{k}^2 t}{2}\right)$$

$$\Psi^P_{\vec{k}}(\vec{r}, 0) = \exp\left(i\vec{k} \cdot \vec{r}\right)$$

Derivatives with respect to $\vec{k}$ produce solutions which at $t = 0$ may have arbitrary polynomial prefactors

$$\Psi^W_{\vec{k}}(\vec{r}, 0) = W(x, y, z) \exp\left(i\vec{k} \cdot \vec{r}\right)$$

Quantum entanglement of vortices

Two straight vortex line along z-axis and x-axis

$$W(x, y, z) = (x + iy)(y + iz)$$

Multiple differentiations produce entanglement

$$[(x + iy)(y + iz)]\, e^{i\vec{k}\cdot\vec{r}} = \left[(-i\frac{\partial}{\partial k_x} + \frac{\partial}{\partial k_y})(-i\frac{\partial}{\partial k_y} + \frac{\partial}{\partial k_z})\right] e^{i\vec{k}\cdot\vec{r}}$$

This initial state evolves into

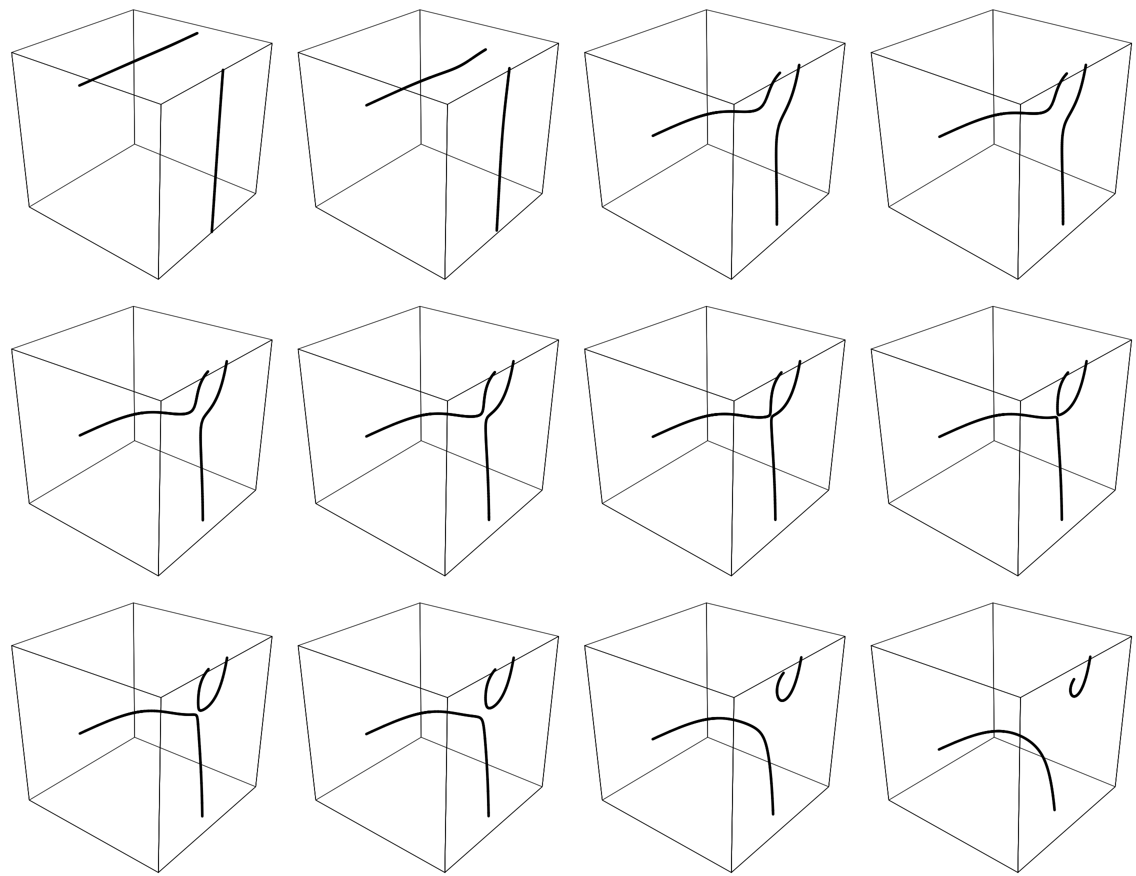
$$\left[((x - v_x t) + i(y - v_y t))\,((y - v_y t) + i(z - v_z t)) - \frac{i\hbar t}{m}\right] e^{i\vec{k}\cdot\vec{r} - i\hbar/2m\vec{k}^2 t}$$

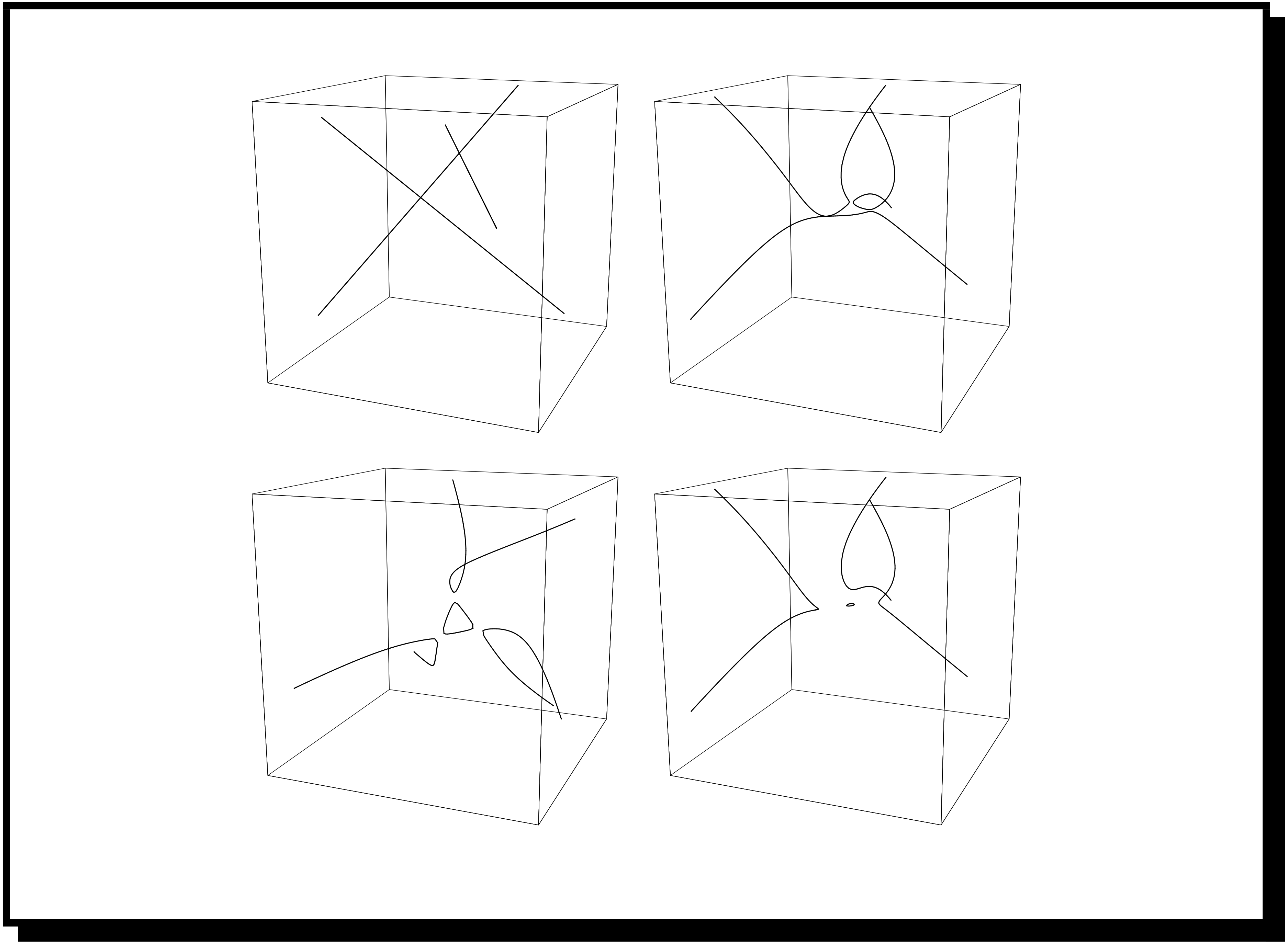
$$\vec{v} = \hbar/m\vec{k}$$

Reconnection of vortices

Reconnection of vortices occurs
when moving vortices cross their paths
Various types of vortex reconnections may be seen:
from simple reconnection of two vortices to
more complicated reconnections of several vortices

Reconnection is a local merging of two vortices





Manufacturing knotted solutions 2

Take the Gaussian solution of the Schrödinger equation

$$\Psi^G_{\vec{k}}(\vec{r},t) = \frac{\exp(-\vec{k}^2 l^2/2)}{(1+i\hbar t/ml^2)^{3/2}} \exp\left[-\frac{(\vec{r}-i\vec{k}l^2)^2}{2l^2(1+i\hbar t/ml^2)}\right]$$

$$\Psi^G_{\vec{k}}(\vec{r},0) = \exp\left(i\vec{k}\cdot\vec{r}\right)\exp\left(-\frac{\vec{r}^2}{2l^2}\right)$$

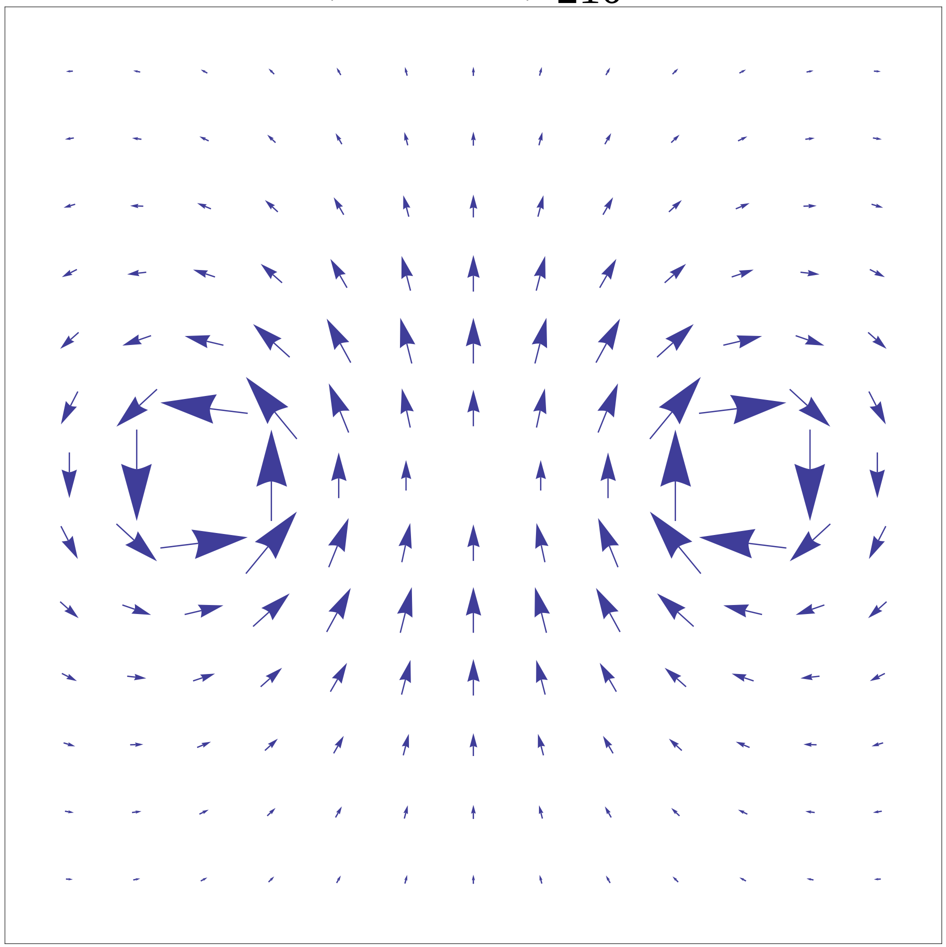
In general, whenever we can solve the Schrödinger equation (without or with a potential) for the initial data

$$\Psi^X_{\vec{k}}(\vec{r},0) = \exp\left(i\vec{k}\cdot\vec{r}\right)\Psi^X(\vec{r})$$

we will be able to generate solutions with vortices

Smoke ring in hydrogen from 2S and 2P states

$\psi_{200} + \mathrm{i}\psi_{210}$



Open problems

- What polynomial produces the trefoil knot?
- What happens when R_3 is replaced by S_3?
- Can all the knots be generated from polynomials?
- How to produce knotted wave functions experimentally?