Massively parallel split step Fourier techniques for simulating quantum systems

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OIST

Overview

This project has created fast, GPU-accelerated software for the simulation of superfluid systems

$$\mathrm{GP}\binom{\hat{U}}{E}$$

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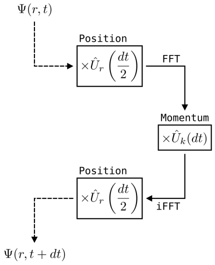

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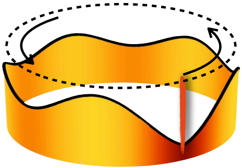

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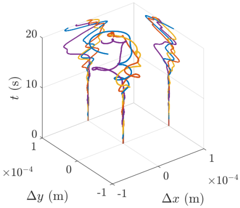

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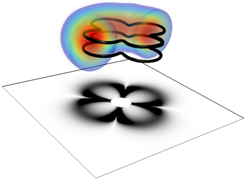

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- Vortex rings with artificial magnetic fields
- Conclusions and future directions

The split-step Fourier method

Heisenberg uncertainty principle

Position and momentum space are conjugate variables

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

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We can flip between spaces with a Fourier transform

The Fourier Transform

Fourier Transform:

$$F(\xi) = \int_{-\infty}^{\infty} f(x) e^{2\pi i x \xi} dx$$

$$f(x) = \int_{-\infty}^{\infty} F(\xi) e^{-2\pi i x \xi} d\xi$$

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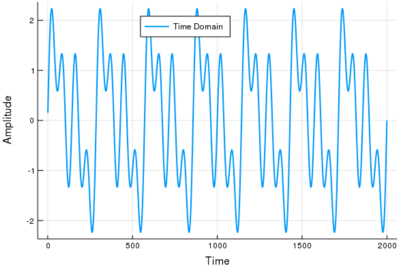

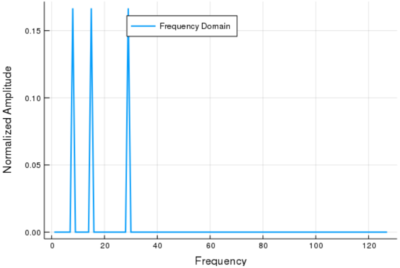

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Discrete Fourier Transform:

$$X_k = \sum_{n=0}^{N-1} x_n e^{2\pi i k x / N}$$

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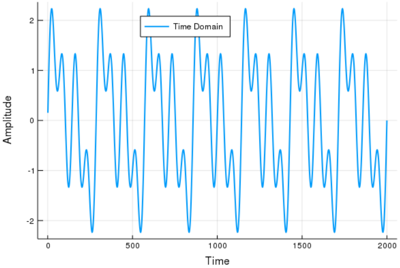

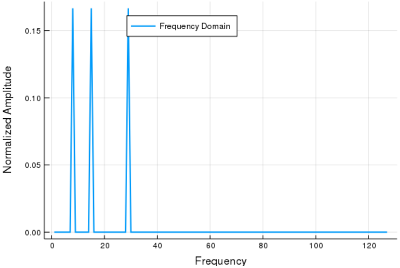

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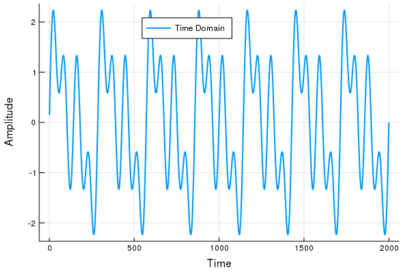
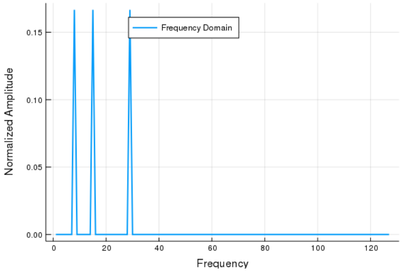
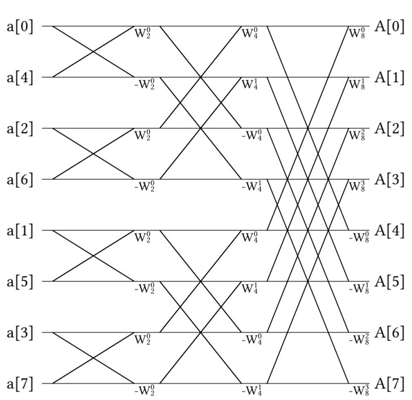
This is a *global* operation requiring matrix multiplications





Cooley-Tukey

- Recursively subdivides DFT into simple sums with twiddle factors
- Many known libraries, like FFTW, and CuFFT
- Hard to parallelize (note for later)



Hamiltonian

1D Schrödinger equation:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left(\frac{\hat{p}^2}{2m} + V_0(\mathbf{r})\right)\Psi(\mathbf{r},t) = \hat{\mathcal{H}}\Psi(\mathbf{r},t)$$

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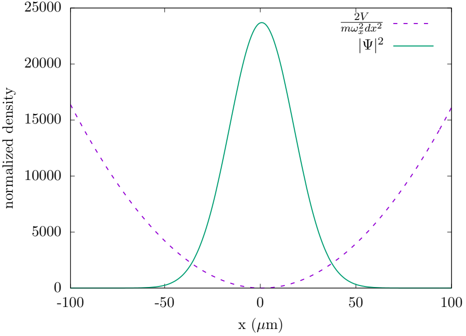
Splits into:

$$\hat{\mathcal{H}}_v = V_0(\mathbf{r}) = \frac{1}{2}m\omega^2x^2$$

$$\hat{\mathcal{H}}_p = \frac{\hat{p}^2}{2m}$$



The Split-Step Fourier Method

Solution for Ψ:

$$\Psi(\mathbf{r}, t + dt) = \left[e^{-\frac{i\hat{\mathcal{H}}dt}{\hbar}}\right] \Psi(\mathbf{r}, t) = \left[e^{-\frac{i(\hat{\mathcal{H}}_v + \hat{\mathcal{H}}_p)dt}{\hbar}}\right] \Psi(\mathbf{r}, t)$$

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$$\Psi(\mathbf{r}, t + dt) = \left[e^{-\frac{i\hat{\mathcal{H}}_V dt}{\hbar}} e^{-\frac{i\hat{\mathcal{H}}_p dt}{\hbar}} e^{-\frac{[i\hat{H}_V, i\hat{H}_p]dt^2}{2}} \right] \Psi(\mathbf{r}, t)$$

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Strang splitting:

$$\Psi(\mathbf{r}, t + dt) = \left[e^{-\frac{i\hat{\mathcal{H}}_V dt}{2\hbar}} e^{-\frac{i\hat{\mathcal{H}}_p dt}{\hbar}} e^{-\frac{i\hat{\mathcal{H}}_V dt}{2\hbar}} \right] \Psi(\mathbf{r}, t) + \mathcal{O}(dt^3)$$

The Split-Step Fourier Method

$$\Psi(\mathbf{r}, t + dt) = \left[\hat{U}_r(dt)\mathcal{F}^{-1}\left[\hat{U}_p(dt)\mathcal{F}\left[\hat{U}_r(dt)\Psi(\mathbf{r}, t)\right]\right]\right] + \mathcal{O}(dt^3)$$

$$\hat{U}_r = e^{-\frac{i\hat{\mathcal{H}}_V dt}{2\hbar}}$$

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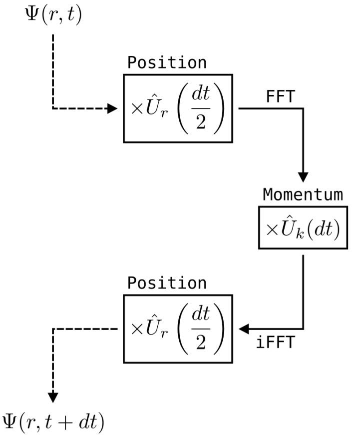
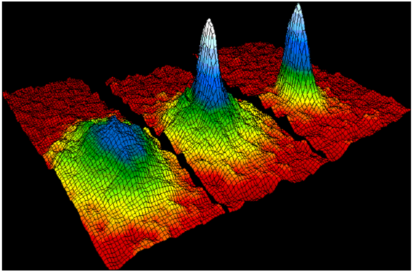


Bose-Einstein condensation

Bosons condense into a superfluid at 0 Kelvin



NIST/JILA/CU-Boulder

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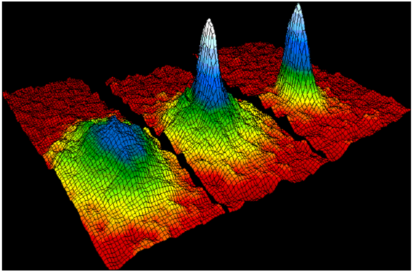


NIST/JILA/CU-Boulder

Described by the Gross–Pitaevskii equation:

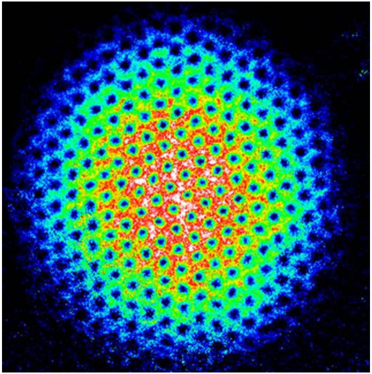
$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2\right)\Psi(\mathbf{r},t).$$

Superfluid rotation

Rotation leads to many vortices in a triangular lattice

Credit: howstuffworks.com

$\rightarrow$



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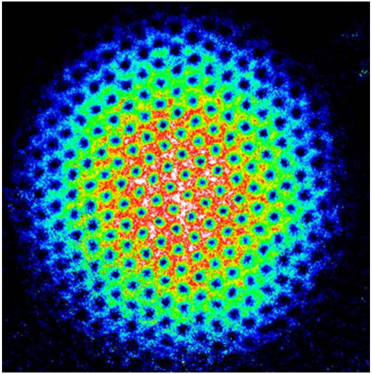

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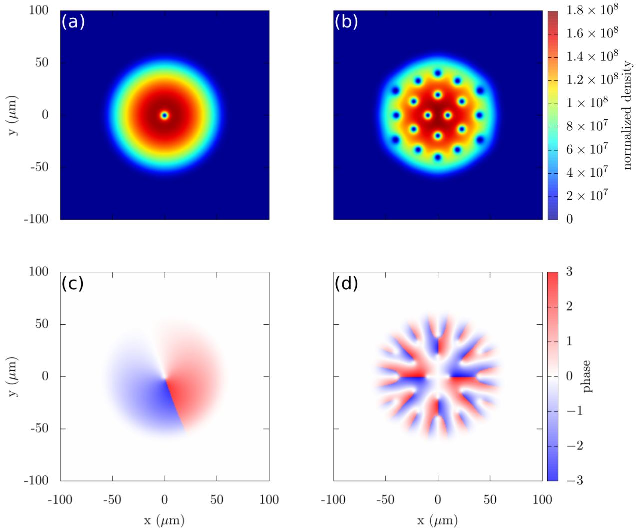
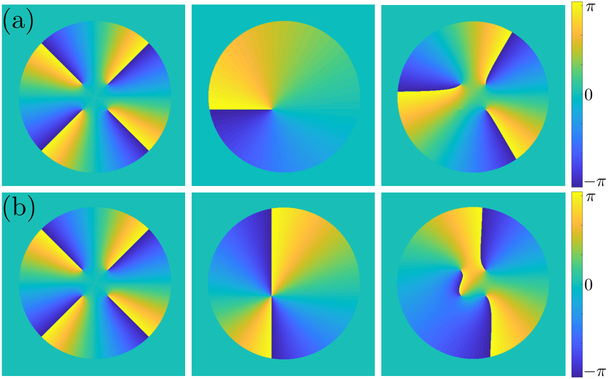
Note: Vortices must follow axis of rotation

Superfluid vortex phase



Each vortex has a 2π complex phase winding

Phase imprinting



Phase masks can induce dynamical vortices

Artificial magnetic fields

Magnetic fields cause rotation in *charged* particles

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- If a two-level atom moves slowly in a tuned light field, *Berry's connection* is

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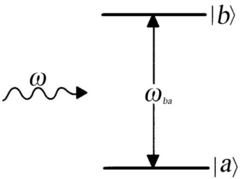
- The magnetic field is

$$\mathbf{B} = \nabla \times \mathbf{A}$$



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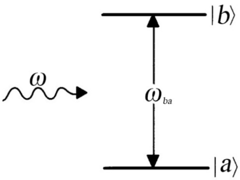
- Vortices follow the magnetic field lines



Modifications to the GPE

With gauge fields, the GPE becomes

$$\hat{\mathcal{H}} = \frac{(p - m\mathbf{A})^2}{2m} + V_0 + g|\Psi(\mathbf{r}, t)|^2$$

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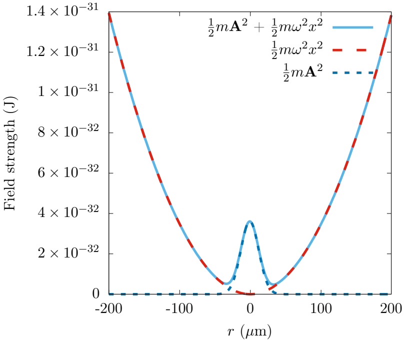

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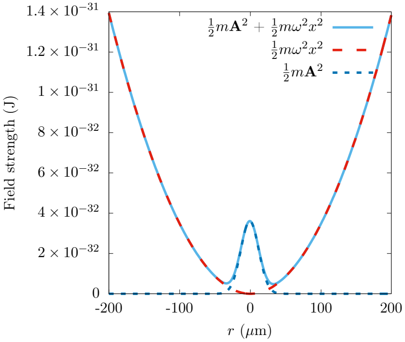
- Components in position and momentum-space, that **require 1D FFT's**

$$-\left(\frac{p\mathbf{A} + \mathbf{A}p}{2}\right)$$



Quantum state engineering

Quantum optimal control

Overall goal: optimize cost function by twiddling control parameters

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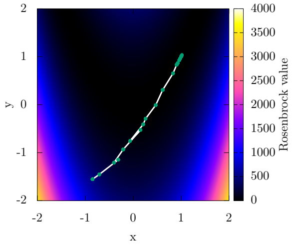
Nelder–Mead

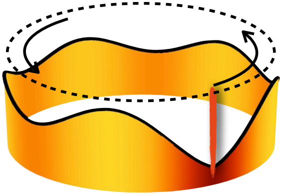


ADD ANIMATION

HELP

Example Tonks–Girardeau gas system

- NOON state: $|N, 0\rangle + |0, N\rangle$
- Tonks–Girardeau Gas: $g \to \infty$



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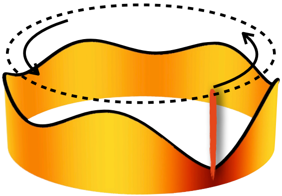
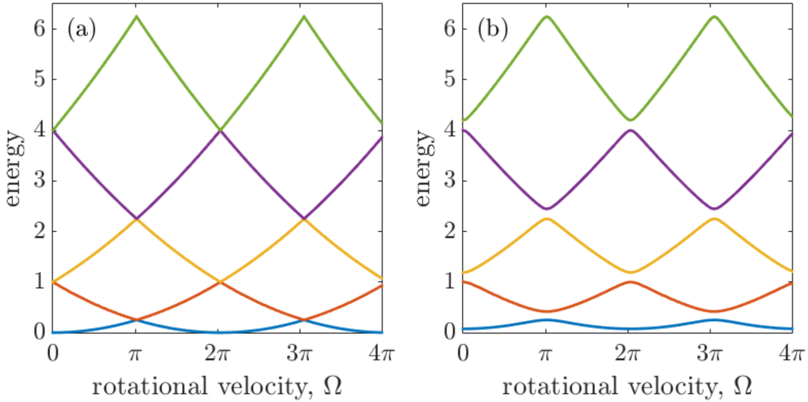




CRAB method

An example protocol is the Chopped RAndom Basis (CRAB) optimal control method where...

- A control parameter is modified with

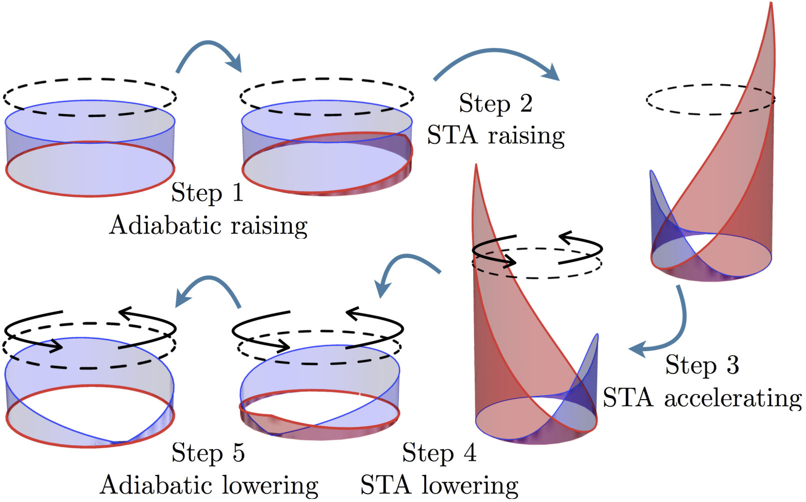
$$\Gamma^{\mathrm{CRAB}}(t) = \Gamma^{0}(t)\gamma(t)$$

  where

$$\gamma(t) = 1 + \frac{1}{\lambda(t)} \sum_{j=1}^{J} (A_j \sin(\nu_j t) + B_j \cos(\nu_j t))$$

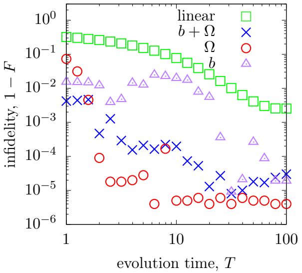
- Works if $\lim_{t\to 0} \lambda(t) = \lim_{t\to T} \lambda(t) = \infty$
- Creates a $3J$-dimensional space to optimize (A, B, ν)

STA protocol



NOON optimization

Optimal control



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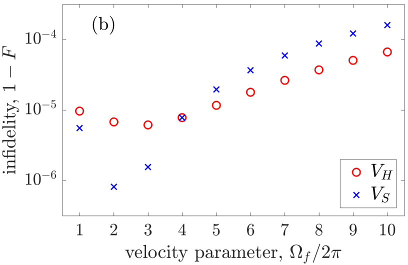

Please ask questions at the end!

GPU computing and the GPUE codebase

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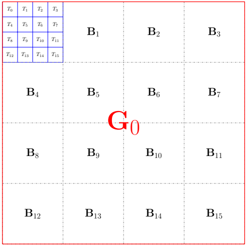
- Computing threads in blocks, blocks in grids



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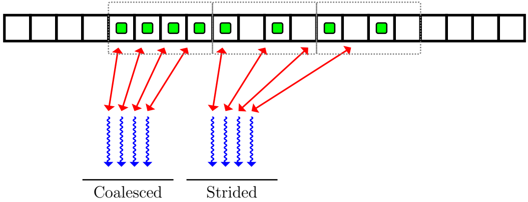

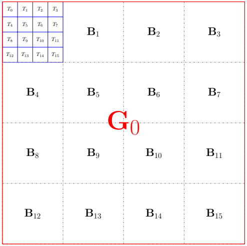

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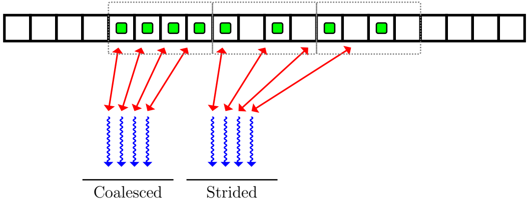
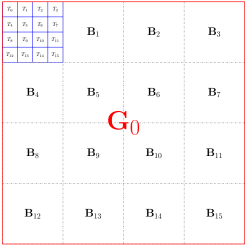
- Data transfer is slow





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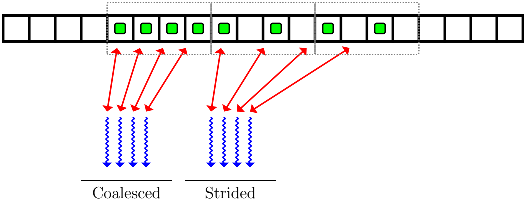

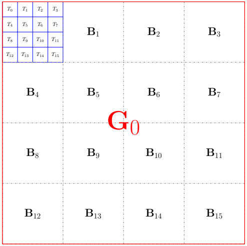

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- Massively parallel computing device
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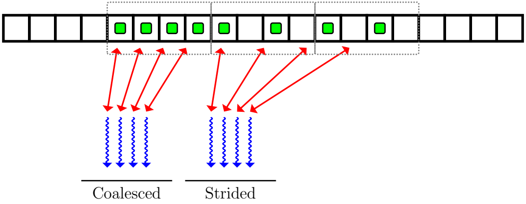
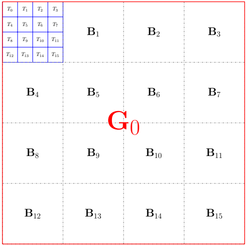
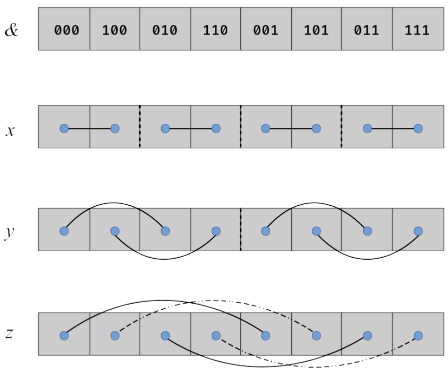
- Data transfer is slow
- Recursion and iteration is slow
- Limited memory

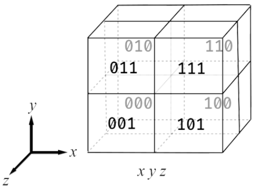




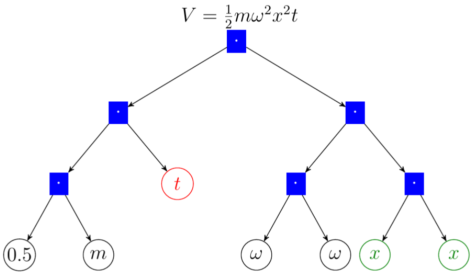
FFT notes

- Global operations
- 1D FFT's are not supported by CuFFT
- Transposes are necessary





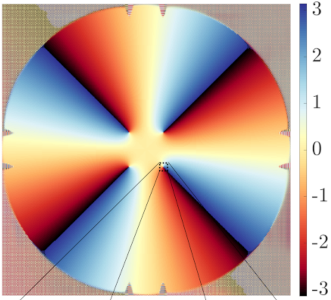
Expression trees



- Allows for quantum state engineering
- Saves GPU memory

Vortex tracking and highlighting

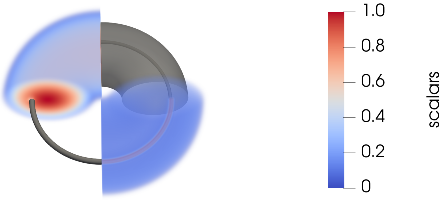
- Phase plaquettes in 2D

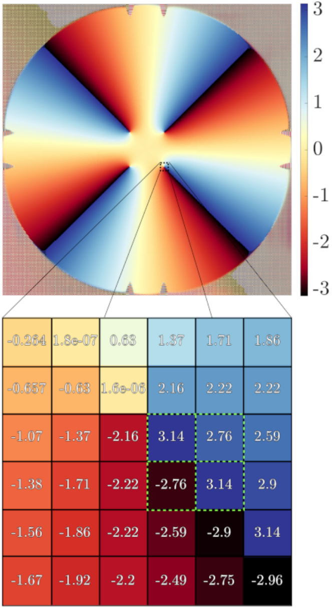


-0.264	1.8e-07	0.63	1.37	1.71	1.86
-0.657	-0.63	1.6e-06	2.16	2.22	2.22
-1.07	-1.37	-2.16	3.14	2.76	2.59
-1.38	-1.71	-2.22	-2.76	3.14	2.9
-1.56	-1.86	-2.22	-2.59	-2.9	3.14
-1.67	-1.92	-2.2	-2.49	-2.75	-2.96

Vortex tracking and highlighting

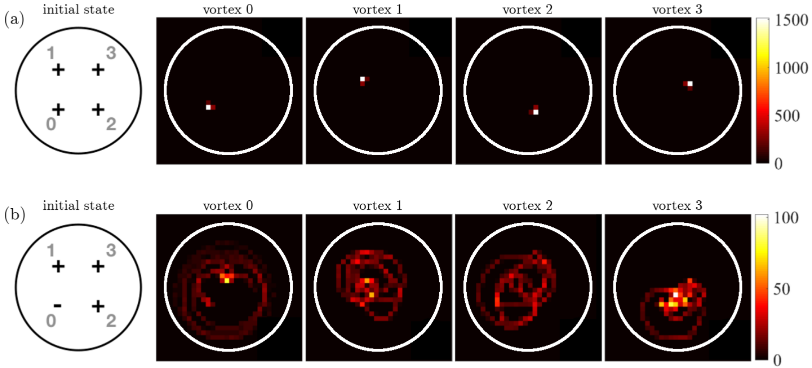
- Phase plaquettes in 2D
- Vortex highlighting in 3D





Chaotic vortex dynamics in 2D BEC simulations

3 vortex, 1 anti-vortex



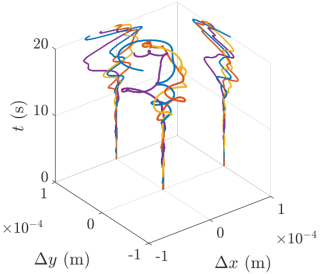
dynamics

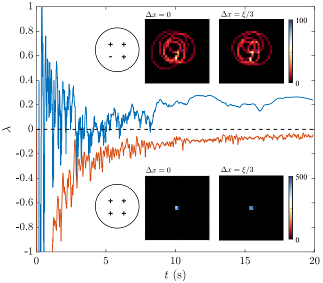
Divergence in trajectories

Divergence in trajectory when Lyapunov exp (λ) becomes positive

$$|\delta \mathbf{P}(t)| \approx e^{\lambda t}|\delta \mathbf{P}_0|$$

$$\lambda = \lim_{t\to\infty} \frac{1}{t}\ln\frac{||\delta \mathbf{P}(t)||}{||\delta \mathbf{P}(0)||}$$

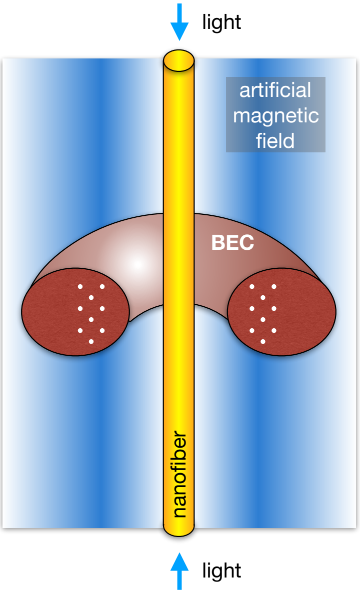




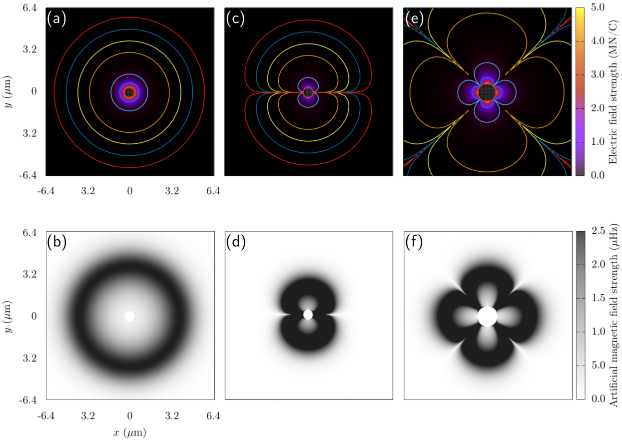
3D vortex ring generation in toroidal BEC systems

The system

- BEC toroidally trapped around nanofiber
- Nanofiber generates $\mathbf{A}$
- Vortices follow $\mathbf{B} = \nabla \times \mathbf{A}$

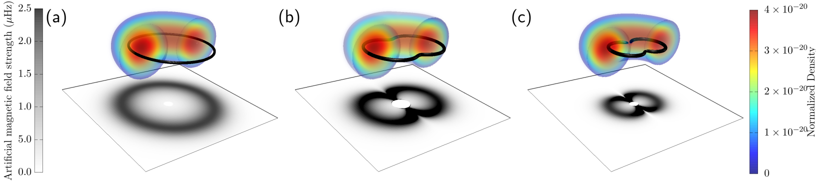


Optical nanofiber

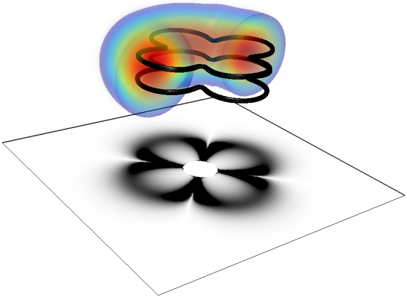


$$\mathbf{A} = \hat{z}\hbar\kappa_0(n_1 + 1)\tilde{s}\left[\frac{|d_r E_r + d_\phi E_\phi + d_z E_z|^2}{1 + \tilde{s}^2|d_r E_r + d_\phi E_\phi + d_z E_z|^2}\right]$$

Vortex structures

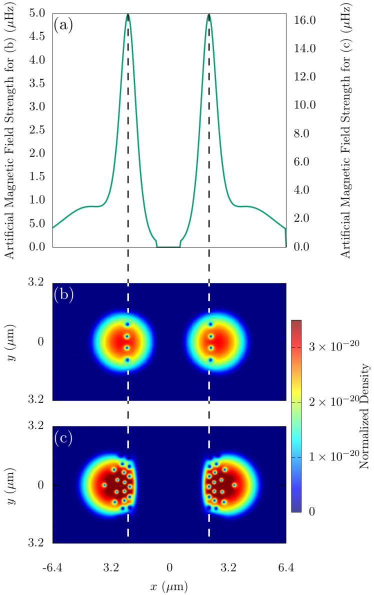


- Transition with linear polarization
- Vortex structures align with **B**



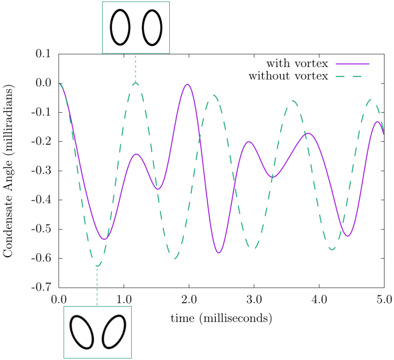
Interesting notes

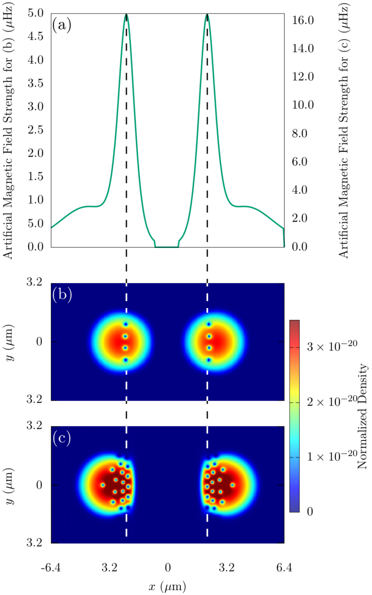
- A vortex ring lattice can be generated with high **B**



Interesting notes

- A vortex ring lattice can be generated with high **B**
- Scissors modes can be used to detect vortices





Overall conclusions

Overall conclusions

- The SSFM is nice
- Quantum state engineering is cool
- GPU computing is fast
- We can create chaos
- We can create not-chaos

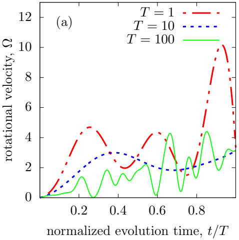
People

- Collaborators: Lee, Rashi, Angela, TT, Andreas, Peter, Albert, Jeremie, Ben, Irina, **Thomas**
- Sponsors: JSPS, OIST, SCDA
- Other: AAA

Conclusions

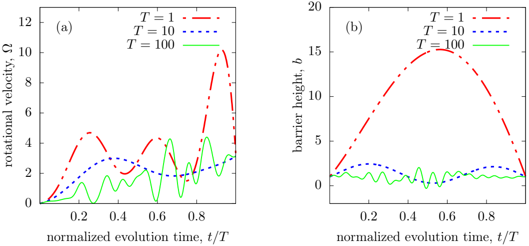
Fidelities with optimal control

- Rotation ($\Omega(t)$)



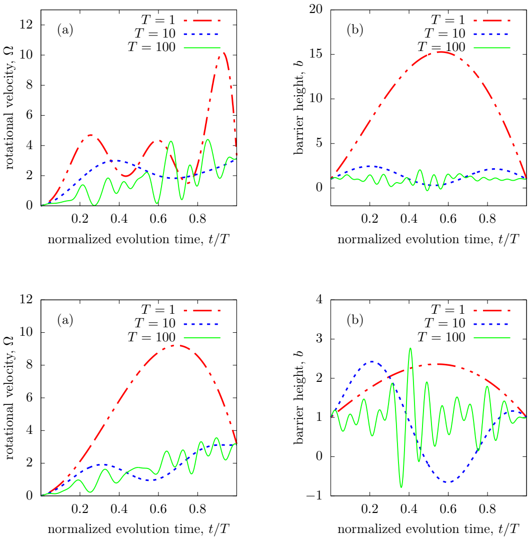
Fidelities with optimal control

- Rotation ($\Omega(t)$)
- Barrier height ($b(t)$)



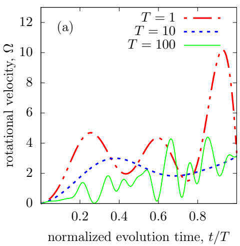
Fidelities with optimal control

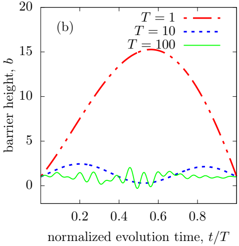
- Rotation ($\Omega(t)$)
- Barrier height ($b(t)$)
- Both

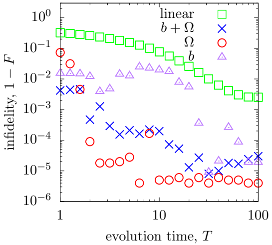


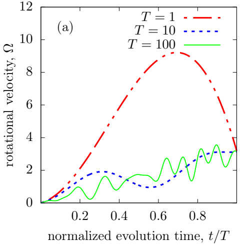
Fidelities with optimal control

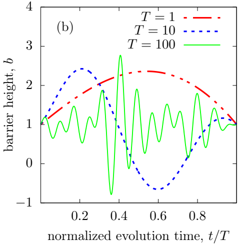
- Rotation ($\Omega(t)$)
- Barrier height ($b(t)$)
- Both





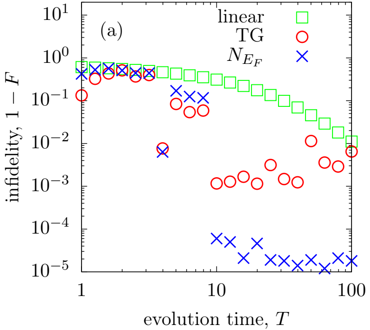




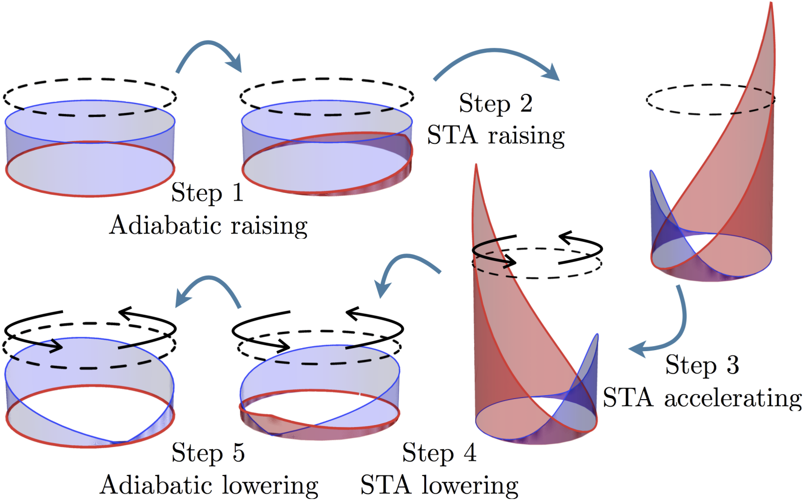


NOON Optimization

Optimizations of NOON state generation with 3 and 5 particles

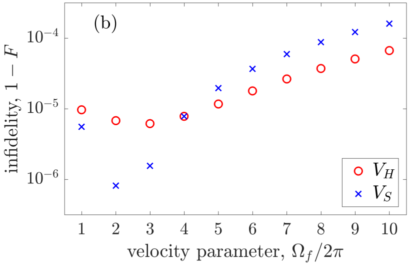


STA protocol



STA fidelities

- Fidelities with rotation



STA fidelities

- Fidelities with rotation
- Fidelities with rotation of 100, 200 and higher particle number