Numerical simulation of vortices

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Outline

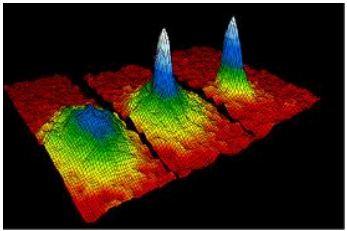
- Introduction: Rotating condensates
- Numerical algorithms for solving Gross-Pitaevskii equation
- Ground state of rotating condensates
- Vortex quantization and generation
- Spin-orbit-coupled condensates

Download: Exercise problems

Useful general reference: A. Fetter, Rev. Mod. Phys. **81**, 647 (2009)

Bose-Einstein condensation

- Intensive progress in the field of ultracold atoms has been recognized by 2001 Nobel prize for experimental realization of Bose-Einstein condensation in 1995
- Cold alkali atoms: Rb, Na, Li, K . . .
  $T \sim 1\,\mathrm{nK}$, $\rho \sim 10^{14}\,\mathrm{cm}^{-3}$
- Cold bosons, cold fermions
- Optical lattices
- Short-range interactions, long-range dipolar interactions, SO coupling, . . .



- Tunable quantum systems concerning dimensionality, type and strength of interactions

Field-theoretical description

- Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$$

- Free Hamiltonian

$$\hat{H}_0 = \int d^3r\, \hat{\Psi}^\dagger(\mathbf{r},t) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r},t)$$

- Interaction

$$\hat{H}_{\text{int}} = \frac{1}{2} \int d^3r \int d^3r'\, \hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r}',t) V_{\text{int}}(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}',t)\hat{\Psi}(\mathbf{r},t)$$

- Bosonic commutation relations

$$\left[\hat{\Psi}(\mathbf{r},t), \hat{\Psi}^\dagger(\mathbf{r}',t)\right] = \delta(\mathbf{r}-\mathbf{r}')\,, \quad \left[\hat{\Psi}(\mathbf{r},t), \hat{\Psi}(\mathbf{r}',t)\right] = \left[\hat{\Psi}^\dagger(\mathbf{r},t), \hat{\Psi}^\dagger(\mathbf{r}',t)\right] = 0$$

- Bogoliubov prescription

$$\hat{\Psi}(\mathbf{r},t) = \Psi(\mathbf{r},t) + \delta\hat{\psi}(\mathbf{r},t)\,, \quad \hat{\Psi}^\dagger(\mathbf{r},t) = \Psi^*(\mathbf{r},t) + \delta\hat{\psi}^\dagger(\mathbf{r},t)$$

Mean-field theory

- Heisenberg equation

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t)=\left[\hat{\Psi}(\mathbf{r},t),\hat{H}\right]$$

- Zeroth order gives mean-field theory

$$\hat{\Psi}(\mathbf{r},t)=\Psi(\mathbf{r},t)\,,\quad \hat{\Psi}^{\dagger}(\mathbf{r},t)=\Psi^{*}(\mathbf{r},t)$$

- Time-dependent Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})+\int d^3r'\,\Psi^{*}(\mathbf{r}',t)V_{\mathrm{int}}(\mathbf{r}-\mathbf{r}')\Psi(\mathbf{r}',t)\right]\Psi(\mathbf{r},t)$$

- Time-independent Gross-Pitaevskii equation

$$\mu\Psi(\mathbf{r})=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})+\int d^3r'\,\Psi^{*}(\mathbf{r}')V_{\mathrm{int}}(\mathbf{r}-\mathbf{r}')\Psi(\mathbf{r}')\right]\Psi(\mathbf{r})$$

Gross-Pitaevskii equation

- Interaction potential: contact interaction, describing s-wave scattering

$$V_{\text{int}}(\mathbf{r}) = g\delta(\mathbf{r}), \quad g = \frac{4\pi\hbar^2 a_s}{m}$$

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- Time-dependent GPE, where we drop the primes

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + gN|\Psi(\mathbf{r}, t)|^2 - \Omega \hat{L}_z \right] \Psi(\mathbf{r}, t)$$

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- $\hat{L}_z = -i\hbar(x\partial/\partial y - y\partial/\partial x)$

Dimensionless form of GPE

- Usually, the trap potential is harmonic

$$V(\mathbf{r}) = \frac{1}{2} m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

- Dimensionless form of GP equation is obtained by rescaling all quantities using convenient units, based on a chosen referent frequency ω_{ref}:
- Length is expressed in units of $\ell = \sqrt{\hbar/(m\omega_{\text{ref}})}$, time in units of $1/\omega_{\text{ref}}$, energy in units of $\hbar\omega_{\text{ref}}$, etc.

$$i\,\frac{\partial \Psi(\mathbf{r},t)}{\partial t} = \left[-\frac{1}{2}\nabla^2 + \frac{1}{2}\left(\gamma^2 x^2 + \nu^2 y^2 + \lambda^2 z^2\right) + g\,|\Psi(\mathbf{r},t)|^2 + i\Omega\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right]\Psi(\mathbf{r},t)$$

$$\gamma = \omega_x/\omega_{\text{ref}}\,, \quad \nu = \omega_y/\omega_{\text{ref}}\,, \quad \lambda = \omega_z/\omega_{\text{ref}}\,, \quad g = 4\pi N a/\ell\,, \quad \tilde{\Omega} = \Omega/\omega_{\text{ref}} \to \Omega$$

Emergence of vortices

Solving GP equation

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$$\mathcal{L}(\Psi^*, \Psi) = \frac{i}{2}\left(\Psi^*\dot{\Psi} - \Psi\dot{\Psi}^*\right) - \frac{1}{2}\nabla\Psi^* \cdot \nabla\Psi - V|\Psi|^2 - \frac{g}{2}|\Psi|^4 - \Omega\Psi^*\hat{L}_z\Psi$$

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- In general, GPE cannot be solved analytically
  - Perturbation methods
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- Many popular numerical methods
  - Split-step methods
  - Finite difference methods
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- Many popular numerical methods
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  - Spectral methods
- **Semi-implicit split-step Crank-Nicolson scheme**
  - Unconditionally stable
  - Preserves normalization of the wave function
  - The error is second order in space and time steps

Split-step Crank-Nicolson method

- GPE in a dimensionless form

$$i\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=\left[-\frac{1}{2}\nabla^2+\frac{1}{2}\left(\gamma^2x^2+\nu^2y^2+\lambda^2z^2\right)+g\left|\Psi(\mathbf{r},t)\right|^2+i\Omega\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\right]\Psi(\mathbf{r},t)$$

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$$t \longrightarrow 2t\,, \quad \tilde{g} = 2g \longrightarrow g\,, \quad \tilde{\Omega} = 2\Omega \longrightarrow \Omega$$

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- Split-step approach

$$\begin{aligned}\hat{H} &= \hat{H}_1+\hat{H}_2+\hat{H}_3+\hat{H}_4\\ \hat{H}_1 &= H_1=\gamma^2x^2+\nu^2y^2+\lambda^2z^2+g|\Psi(\mathbf{r},t)|^2\\ \hat{H}_2 &= -\frac{\partial^2}{\partial x^2}-i\Omega y\frac{\partial}{\partial x}\,,\quad \hat{H}_3=-\frac{\partial^2}{\partial y^2}+i\Omega x\frac{\partial}{\partial y}\,,\quad \hat{H}_4=-\frac{\partial^2}{\partial z^2}\end{aligned}$$

Comput. Phys. Commun. **180**, 1888 (2009); Comput. Phys. Commun. **240**, 74 (2019)

Split-step Crank-Nicolson method (non-rotating case)

- Propagate GPE from t_n ($t_n = n\Delta$) to t_{n+1} in multiple steps

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$$\hat{H}_2\Psi^m_{i,j,k} = \frac{\Psi^m_{i+1,j,k} - 2\Psi^m_{i,j,k} + \Psi^m_{i-1,j,k}}{h_x^2}, \quad \Psi^m_{i,j,k} \equiv \Psi(x_i, y_j, z_k, t_m), \quad x_i = \left(i - \frac{N_x}{2}\right)h_x, \ldots$$

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- Resulting tridiagonal eqs. are solved using forward recursion and backward substitution
- Propagation wrt $\hat{H}_3$ yields $\Psi^{n+1/2+2/6}$, and wrt $\hat{H}_4$ gives $\Psi^{n+1/2+3/6} = \Psi^{n+1}$

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- Chemical potential is calculated as

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Available software packages

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    - Comput. Phys. Commun. **220**, 503 (2017): Fortran/OpenMP
  - **BEC-GP-ROT** (rotation and contact interaction):
    - Comput. Phys. Commun. **240**, 74 (2019): Fortran/OpenMP, C/OpenMP

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  - **BEC-GP-SPINOR-ROT** (rotation, contact interaction and SO coupling)
    - Comput. Phys. Commun. **264**, 107926 (2021): Fortran/OpenMP

Shared memory algorithm on multi-core CPUs - OpenMP

- Propagation wrt H_1 is easy to parallelize
- How to parallelize the CN method?

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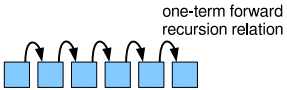

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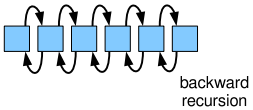

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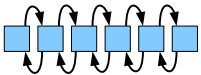
- How to parallelize the CN method?
  - Difficult due to recursion calculation



difficult to parallelize

Shared memory algorithm on multi-core CPUs - OpenMP

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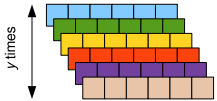

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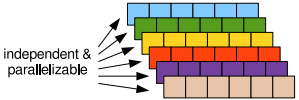

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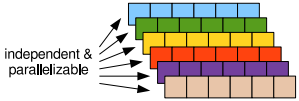
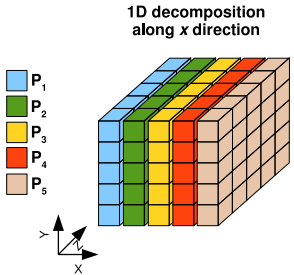


- Solution:
  - Parallelize outermost loop (with OpenMP)
  - This uses more memory due to thread-private variables (arrays)

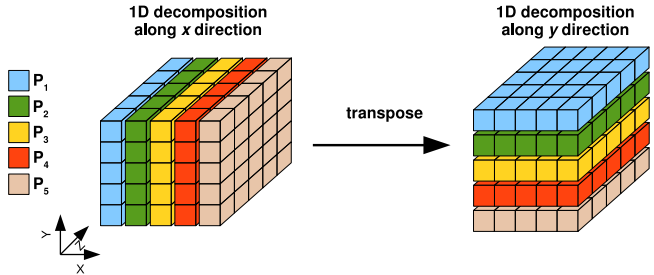
Distributed memory algorithm - OpenMP/MPI

- 1D decomposition



Distributed memory algorithm - OpenMP/MPI

- 1D decomposition
  - Dynamically redistribute data via transpose operation
  - Use existing computation routines to work with local data
  - Two ways to transpose data, via FFTW or via our function



Our experimental equipment

- PARADOX-IV cluster
  - Each node has 2 × Intel Xeon E5-2670
    - $2 \times 8 = 16$ cores
    - 32 GB RAM
  - Each node has Nvidia Tesla M2090 GPU
    - 512 CUDA cores
    - 6 GB RAM
    - Fermi architecture
    - Compute Capability 2.0
- 1696 CPU cores, 106 GPU cards

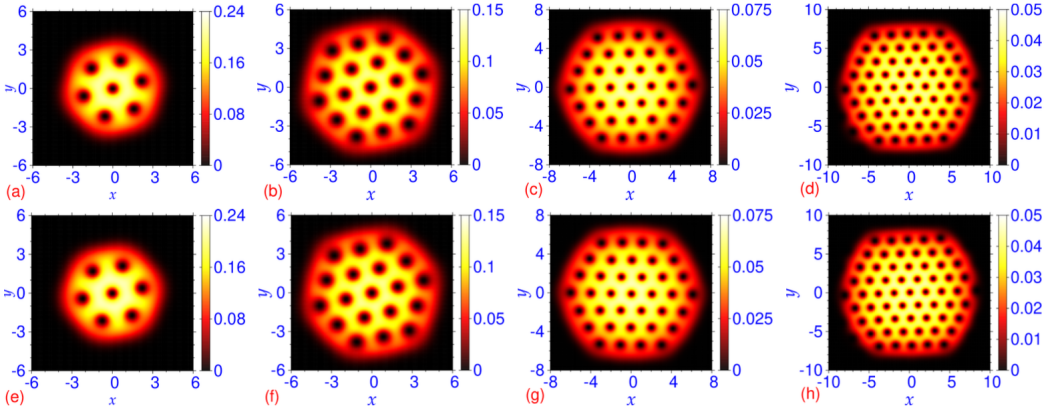
Numerical calculation of the ground state

- We consider a pancake-shaped condensate: $\gamma = \nu = 1$, $\lambda = 100$
- Nonlinearity: $g = 25.066283$
- Discretization grid: $N_x = N_y = 256$, $N_z = 32$; for $\Omega \geq 0.9$, $N_x = N_y = 512$
- Grid spacing: $h_x = h_y = 0.05$, $h_z = 0.025$
- Initial state:

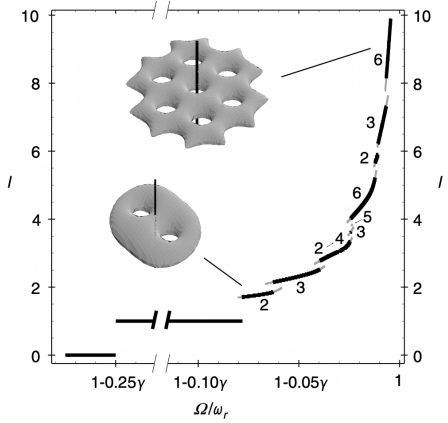
$$\phi_{\rm in}(x,y) = \frac{x+iy}{\sqrt{\pi d_x d_y}} \exp\left(-\frac{x^2}{2d_x^2} - \frac{y^2}{2d_y^2} + 2\pi i \mathcal{R}(x,y)\right), \quad \psi_{\rm in}(x,y,z) = \phi_{\rm in}(x,y) \frac{1}{(\pi d_z^2)^{1/4}} \exp\left(-\frac{z^2}{2d_z^2}\right)$$

- Visualization of density profiles: VisIt
- **BEC-GP-ROT**: Comput. Phys. Commun. **240**, 74 (2019)
- C/OpenMP/MPI program available at: http://www.scl.rs/IWeek2022/

Fast-rotating condensates

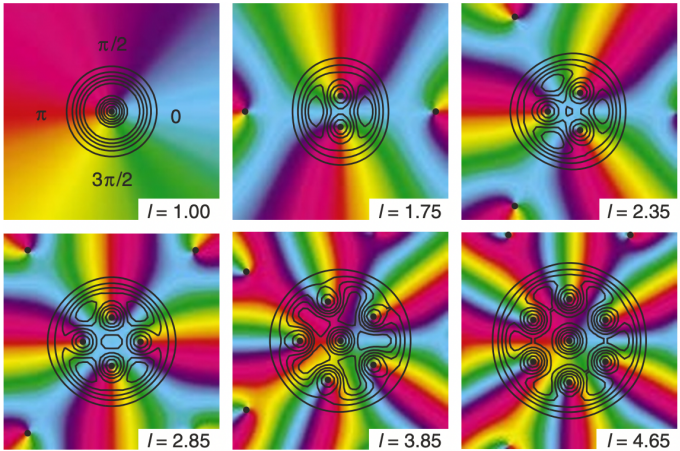


Vortices and quantization of angular momentum



Butts & Rokhsar, Nature **397**, 327 (1999)

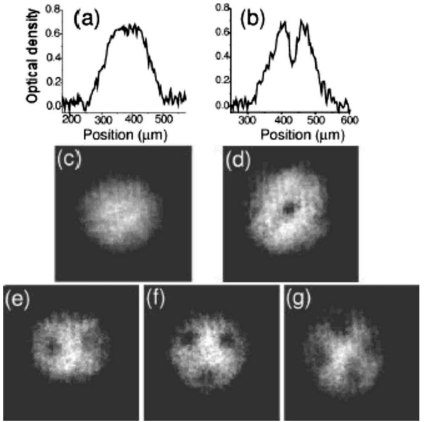
Phase profile of vortex structure



Butts & Rokhsar, Nature **397**, 327 (1999)

Experimental and numerical techniques for vortex generation

- Rotation (fast enough)
- Laser stirring
- Phase imprinting: $e^{im\varphi}$
- Moving obstacle



Dalibard group, Phys. Rev. Lett. **84**, 806 (2000)

Moving obstacle: emergence of vortices

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SO-coupled condensates

$$i\partial_t\psi_{\pm1}(\mathbf{r}) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{r}) + c_0\rho + c_2\left(\rho_{\pm1} - \rho_{\mp1} + \rho_0\right)\right]\psi_{\pm1}(\mathbf{r}) + \left\{c_2\psi_0^2(\mathbf{r})\psi_{\mp1}^*(\mathbf{r})\right\} + \frac{\Omega}{\sqrt{2}}\psi_0(\mathbf{r}) + \gamma f_{\pm1}$$

$$i\partial_t\psi_0(\mathbf{r}) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{r}) + c_0\rho + c_2\left(\rho_{+1} + \rho_{-1}\right)\right]\psi_0(\mathbf{r}) + \left\{2c_2\psi_{+1}(\mathbf{r})\psi_{-1}(\mathbf{r})\psi_0^*(\mathbf{r})\right\} + \frac{\Omega}{\sqrt{2}}\sum_{j=+1,-1}\psi_j(\mathbf{r}) + \gamma g$$

$$\rho_j = |\psi_j|^2\,, \quad \int\left[\rho_{+1}(\mathbf{r}) + \rho_0(\mathbf{r}) + \rho_{-1}(\mathbf{r})\right]d\mathbf{r} = 1\,, \quad \int\left[\rho_{+1}(\mathbf{r}) - \rho_{-1}(\mathbf{r})\right]d\mathbf{r} = m$$

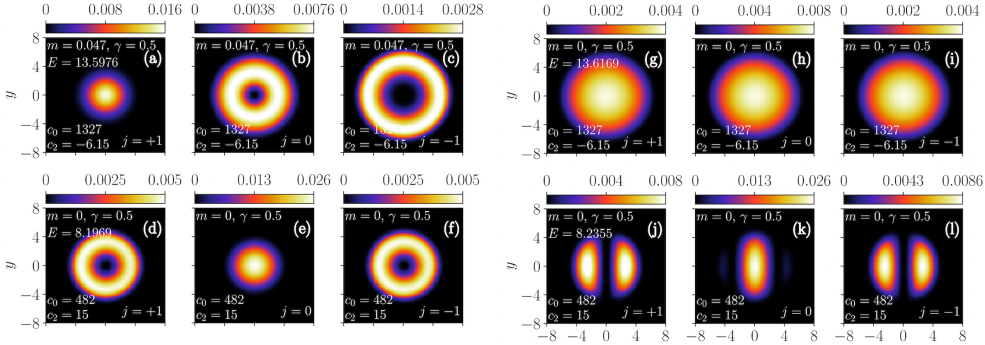
- SO coupling: $\gamma(\eta p_y\Sigma_x - p_x\Sigma_y)$, where $\eta = 1, -1, 0$ for Rashba, Dresselhaus and an equal mixture

$$\Sigma_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \Sigma_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \Sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

$$\gamma f_{\pm1} = -i\widetilde{\gamma}\left[\eta\partial_y\psi_0(\mathbf{r}) \pm i\partial_x\psi_0(\mathbf{r})\right], \quad \gamma g = -i\widetilde{\gamma}\left[-i\partial_x\psi_{+1}(\mathbf{r}) + i\partial_x\psi_{-1}(\mathbf{r}) + \eta\partial_y\psi_{+1}(\mathbf{r}) + \eta\partial_y\psi_{-1}(\mathbf{r})\right]$$

SO-coupled condensates

- **BEC-GP-SPINOR** (contact interaction and SO coupling)
  - Comput. Phys. Commun. **259**, 107657 (2021): Fortran/OpenMP



SO-coupled rotating condensates

- **BEC-GP-SPINOR-ROT** (rotation, contact interaction and SO coupling)
  - Comput. Phys. Commun. **264**, 107926 (2021): Fortran/OpenMP