Efficient algorithms for the time-dependent Gross-Pitaevskii equation with harmonic potentials

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Summary

- The Gross-Pitaevskii equation
  in 1 and 3 dimensions

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- Spectral method

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  some physical examples

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- Time evolution
  some physical examples
- Conclusion & perspectives

Gross-Pitaevskii equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}} + \frac{4\pi\hbar^2 aN}{m}\left|\psi\right|^2\right]\psi$$

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- Non-linear Schrödinger equation

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- Non-linear Schrödinger equation
- Corresponds to a $T = 0$ K approximation
  All bosons are in the condensed state

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- Non-linear Schrödinger equation
- Corresponds to a $T = 0$ K approximation
  All bosons are in the condensed state
- Been shown to correctly reproduce experimental observations

Gross-Pitaevskii equation

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External (trapping) potential V_{ext} taken to be harmonic

$$V_{\text{ext}} = \frac{1}{2}m\omega_{\mathbf{x}}^2\left|\mathbf{x}\right|^2$$

Rescaling

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega_{\mathbf{x}}^2\left|\mathbf{x}\right|^2 + \frac{4\pi\hbar^2 aN}{m}\left|\psi\right|^2\right]\psi$$

$$\begin{aligned} x &= \left(\frac{\hbar}{m\omega_x}\right)^{1/2} X \\ y &= \left(\frac{\hbar}{m\omega_y}\right)^{1/2} Y \\ z &= \left(\frac{\hbar}{m\omega_z}\right)^{1/2} Z \\ t &= \frac{1}{\omega_x}\tau \end{aligned}$$

Rescaling

$$i\frac{\partial}{\partial \tau}\Psi = \left[H_{0,X} + \frac{\omega_y}{\omega_x}H_{0,Y} + \frac{\omega_z}{\omega_x}H_{0,Z} + \lambda\left|\Psi\right|^2\right]\Psi$$

$$H_{0,X} = -\frac{1}{2}\nabla^2_X + \frac{X^2}{2}$$

Non-linearity

$$i\frac{\partial}{\partial\tau}\Psi = \left[H_{0,X} + \frac{\omega_y}{\omega_x}H_{0,Y} + \frac{\omega_z}{\omega_x}H_{0,Z} + \lambda\left|\Psi\right|^2\right]\Psi$$

$$\lambda = 4\pi a N\left(\frac{m}{\hbar}\frac{\omega_y\omega_z}{\omega_x}\right)^{1/2}$$

$$\int_{\mathbb{R}^3}\left|\Psi\right|^2 dX\,dY\,dZ = 1$$

Non-linearity

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at the lower end:

^{4}He* ($m = 4.0$ a.m.u., $a = 302$ a.u.), $N = 10^3$

highly anisotropic trap: $\omega_y\omega_z/\omega_x = 2\pi \times 10^{-1}$ Hz

$$\lambda \approx 1.3$$

Non-linearity

$$i\frac{\partial}{\partial\tau}\Psi = \left[H_{0,X} + \frac{\omega_y}{\omega_x}H_{0,Y} + \frac{\omega_z}{\omega_x}H_{0,Z} + \lambda\left|\Psi\right|^2\right]\Psi$$

$$\lambda = 4\pi aN\left(\frac{m}{\hbar}\frac{\omega_y\omega_z}{\omega_x}\right)^{1/2}$$

at the upper end:

^{87}Rb ($m = 86.9$ a.m.u., $a = 106$ a.u.), $N = 10^5$

isotropic trap: $\omega \sim 2\pi \times 10^2$ Hz

$$\lambda \sim 10^5$$

Non-linearity

$$i\frac{\partial}{\partial \tau}\Psi = \left[H_{0,X} + \frac{\omega_y}{\omega_x}H_{0,Y} + \frac{\omega_z}{\omega_x}H_{0,Z} + \lambda \left|\Psi\right|^2\right]\Psi$$

$$\lambda = 4\pi a N \left(\frac{m}{\hbar}\frac{\omega_y \omega_z}{\omega_x}\right)^{1/2}$$

$$\lambda \sim 1 - 10^2$$

$$\lambda > 0$$

Spherical symmetry

$$i\frac{\partial}{\partial\tau}\Psi = \left[H_{0,X} + \frac{\omega_y}{\omega_x}H_{0,Y} + \frac{\omega_z}{\omega_x}H_{0,Z} + \lambda\left|\Psi\right|^2\right]\Psi$$

$$\omega_z = \omega_y = \omega_x$$

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$$\omega_z = \omega_y = \omega_x$$

$$\Psi(R,\theta,\varphi) \equiv \chi(R)\Upsilon(\theta,\varphi)$$

with

$$\Upsilon(\theta,\varphi) = (4\pi)^{-1/2}$$

Spherical symmetry

$$i\frac{\partial}{\partial\tau}\chi = \left[-\frac{1}{2R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right) + \frac{R^2}{2} + \frac{\lambda}{4\pi}\left|\chi\right|^2\right]\chi$$

Spherical symmetry

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$$\tilde{\chi}(R) \equiv R\chi(R)$$

$$i\frac{\partial}{\partial\tau}\tilde{\chi} = \left[-\frac{1}{2}\frac{\partial^2}{\partial R^2} + \frac{R^2}{2} + \frac{\lambda}{4\pi R^2}\left|\tilde{\chi}\right|^2\right]\tilde{\chi}$$

Spectral method

1D: $$i\frac{\partial}{\partial\tau}\tilde{\chi} = \left[H_{0,R} + \frac{\lambda}{4\pi R^2}\left|\tilde{\chi}\right|^2\right]\tilde{\chi}$$

3D: $$i\frac{\partial}{\partial\tau}\Psi = \left[H_{0,X} + \frac{\omega_y}{\omega_x}H_{0,Y} + \frac{\omega_z}{\omega_x}H_{0,Z} + \lambda\left|\Psi\right|^2\right]\Psi$$

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3D: $$i\frac{\partial}{\partial\tau}\Psi = \left[H_{0,X} + \frac{\omega_y}{\omega_x}H_{0,Y} + \frac{\omega_z}{\omega_x}H_{0,Z} + \lambda\left|\Psi\right|^2\right]\Psi$$

$$\Psi(X,Y,Z,\tau) = \sum_{i=0}^{N_X}\sum_{j=0}^{N_Y}\sum_{k=0}^{N_Z} c_{ijk}(\tau)\phi_i(X)\phi_j(Y)\phi_k(Z)$$

$$H_0\phi_n = \left(n + \frac{1}{2}\right)\phi_n$$

Coupled equations

$$i\dot{c}_{ijk} = E_{ijk} c_{ijk} + \lambda \alpha_{ijk}$$

$$E_{ijk} = \left(i + \frac{1}{2}\right) + \frac{\omega_y}{\omega_x}\left(j + \frac{1}{2}\right) + \frac{\omega_z}{\omega_x}\left(k + \frac{1}{2}\right)$$

$$\alpha_{ijk} = \Big(\phi_i(X)\phi_j(Y)\phi_k(Z), \left|\Psi(X,Y,Z)\right|^2 \Psi(X,Y,Z)\Big)$$

Scalar product

$$\alpha_{ijk} = \Big(\phi_i(x)\phi_j(y)\phi_k(z), |\psi(x,y,z)|^2\,\psi(x,y,z)\Big)$$

$$\phi_n(x) = (2^n n!)^{-1/2}\,\pi^{-1/4} H_n(x) e^{-x^2/2}$$

$$\psi(x,y,z) = \sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\sum_{k=0}^{N_z} c_{ijk}\phi_i(x)\phi_j(y)\phi_k(z)$$

Scalar product

$$\alpha_{ijk} = \Big(\phi_i(x)\phi_j(y)\phi_k(z), |\psi(x,y,z)|^2\,\psi(x,y,z)\Big)$$

$$\alpha = \int_{\mathbb{R}^3} \mathcal{P}_{4N_x}(x)e^{-2x^2}\mathcal{P}_{4N_y}(y)e^{-2y^2}\mathcal{P}_{4N_z}(z)e^{-2z^2}dxdydz$$

$$\phi_n(x) = (2^n n!)^{-1/2}\,\pi^{-1/4}H_n(x)e^{-x^2/2}$$

$$\psi(x,y,z) = \sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\sum_{k=0}^{N_z} c_{ijk}\phi_i(x)\phi_j(y)\phi_k(z)$$

Gauss-Hermite quadrature

$$\alpha = 2^{-3/2} \int_{\mathbb{R}^3} \mathcal{P}_{4N_x}(\tilde{x}) e^{-\tilde{x}^2} \mathcal{P}_{4N_y}(\tilde{y}) e^{-\tilde{y}^2} \mathcal{P}_{4N_z}(\tilde{z}) e^{-\tilde{z}^2} d\tilde{x} d\tilde{y} d\tilde{z}$$

$$\begin{aligned} \alpha &= 2^{-3/2} \sum_{l=1}^{2N_x+1} w_{x,l} \mathcal{P}_{4N_x}(\tilde{x}_l) \sum_{m=1}^{2N_y+1} w_{y,m} \mathcal{P}_{4N_y}(\tilde{y}_m) \\ &\quad \times \sum_{n=1}^{2N_z+1} w_{z,n} \mathcal{P}_{4N_z}(\tilde{z}_n) \end{aligned}$$

$\sqrt{2}\tilde{x}_l =$ roots of $H_{2N_x+1} \Longrightarrow 2N_x + 1$ points/dimension
$w_{x,l} =$ corresponding Gauss weights

Algorithm

1. Determine the value of ψ on the Gauss points $\tilde{x}_l$ from the c_{ijk} coefficients

$$f_{ljk} = \sum_i c_{ijk} \phi_i(\tilde{x}_l)$$

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1b. Repeat step (1) for the two other spatial dimensions to obtain

$$f_{lmn} \equiv \psi(\tilde{x}_l, \tilde{y}_m, \tilde{z}_n)$$

Algorithm

1. Determine the value of ψ on the Gauss points $\tilde{x}_l$ from the c_{ijk} coefficients

1b. Repeat step (1) for the two other spatial dimensions to obtain $\psi(\tilde{x}_l, \tilde{y}_m, \tilde{z}_n)$

2. Calculate

$$g_{lmn} = \lambda \left| f_{lmn} \right|^2 f_{lmn} w_{x,l} w_{y,m} w_{z,n}$$

Algorithm

1. Determine the value of ψ on the Gauss points $\tilde{x}_l$ from the c_{ijk} coefficients

1b. Repeat step (1) for the two other spatial dimensions to obtain $\psi(\tilde{x}_l, \tilde{y}_m, \tilde{z}_n)$

2. Calculate $\lambda |\psi|^2 \psi$

3. Transform back to the c_{ijk} coefficients by successive application of

$$f_{imn} = \sum_l g_{lmn} \phi_i(\tilde{x}_l)$$

in the three spatial dimensions.

Algorithm

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$O(N^4)$ method

Advantages

Spectral method *vs* grid methods

- $O(N^{d+1})$ *vs* $O(N^d \log_2 N)$ for FFT methods

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Spectral method *vs* grid methods

- $O(N^{d+1})$ *vs* $O(N^d \log_2 N)$ for FFT methods
- fewer basis functions than grid points
  especially when Ψ has a definite parity
  (only even or odd harmonic oscillator functions are needed)

Time evolution

$$i\dot{c}_{ijk} = E_{ijk}c_{ijk} + \lambda\alpha_{ijk}$$

time propagation from an initial $c_{ijk}(\tau = 0)$ condition

4th order Runge-Kutta scheme

Ground stationary state

$$\left[H_{0,X} + \frac{\omega_y}{\omega_x} H_{0,Y} + \frac{\omega_z}{\omega_x} H_{0,Z} + V_0(X,Y,Z) + \lambda |\Psi|^2 \right] \Psi = \mu \Psi$$

Ground stationary state

$$\left[H_{0,X} + \frac{\omega_y}{\omega_x} H_{0,Y} + \frac{\omega_z}{\omega_x} H_{0,Z} + V_0(X,Y,Z) + \lambda \rho\right] \Psi = \mu \Psi$$

Ground stationary state

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Iterative procedure:

0. Set an initial ρ_0
1. Solve $H(\rho_{i-1})\Psi_i = \mu\Psi_i$
   (find ground state)
2. Construct ρ_i from Ψ_i
3. Iterate until $\rho_i \simeq \rho_{i-1}$

Optimal damping algorithm

Initialization: from $H(\rho_0)$ get $D_{\rm in}$, $D_{\rm in} \longrightarrow \rho_{\rm in}$

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   $\hookrightarrow$ 1D: diagonalize Hamiltonian matrix
   $\hookrightarrow$ 3D: inverse power method + conjugated gradient

Optimal damping algorithm

Initialization: from $H(\rho_0)$ get $D_{\rm in}$, $D_{\rm in} \longrightarrow \rho_{\rm in}$

Optimization:

1. $H(\rho_{\rm in}) \longrightarrow D_{\rm out}$
2. $D_{\rm out} - D_{\rm in}$ “small”?
   yes: converged, no: $D_{\rm out} \longrightarrow \rho_{\rm out}$

Optimal damping algorithm

Initialization: from $H(\rho_0)$ get D_{in}, $D_{\text{in}} \longrightarrow \rho_{\text{in}}$

Optimization:

1. $H(\rho_{\text{in}}) \longrightarrow D_{\text{out}}$
2. $D_{\text{out}} - D_{\text{in}}$ "small"?
   yes: converged, no: $D_{\text{out}} \longrightarrow \rho_{\text{out}}$
3. $D = (1-\gamma)D_{\text{in}} + \gamma D_{\text{out}}$

   γ is optimized at each step by $\gamma = \max\left(-s/2c, 1\right)$

   $s = \text{Tr}\left[H(\rho_{\text{in}}) \cdot D_{\text{out}}\right] - \text{Tr}\left[H(\rho_{\text{in}}) \cdot D_{\text{in}}\right]$

   $c = \text{Tr}\left[H(\rho_{\text{in}}) \cdot D_{\text{in}}\right] + \text{Tr}\left[H(\rho_{\text{out}}) \cdot D_{\text{out}}\right] -$

   $\text{Tr}\left[H(\rho_{\text{in}}) \cdot D_{\text{out}}\right] - \text{Tr}\left[H(\rho_{\text{out}}) \cdot D_{\text{in}}\right]$

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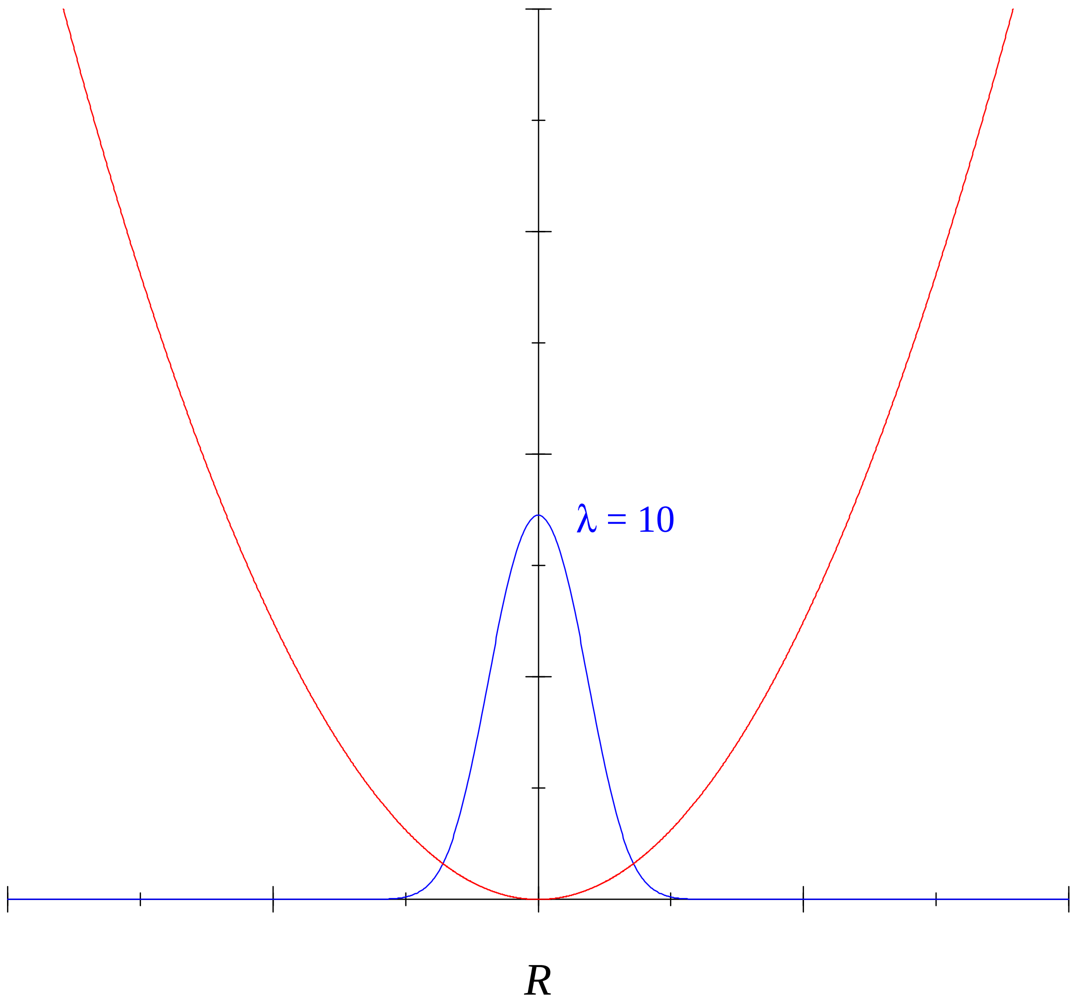
   yes: converged, no: $D_{\text{out}} \longrightarrow \rho_{\text{out}}$
3. $D = (1-\gamma)D_{\text{in}} + \gamma D_{\text{out}}$
4. $D \longrightarrow D_{\text{in}} \longrightarrow \rho_{\text{in}}$, iterate

1D Example



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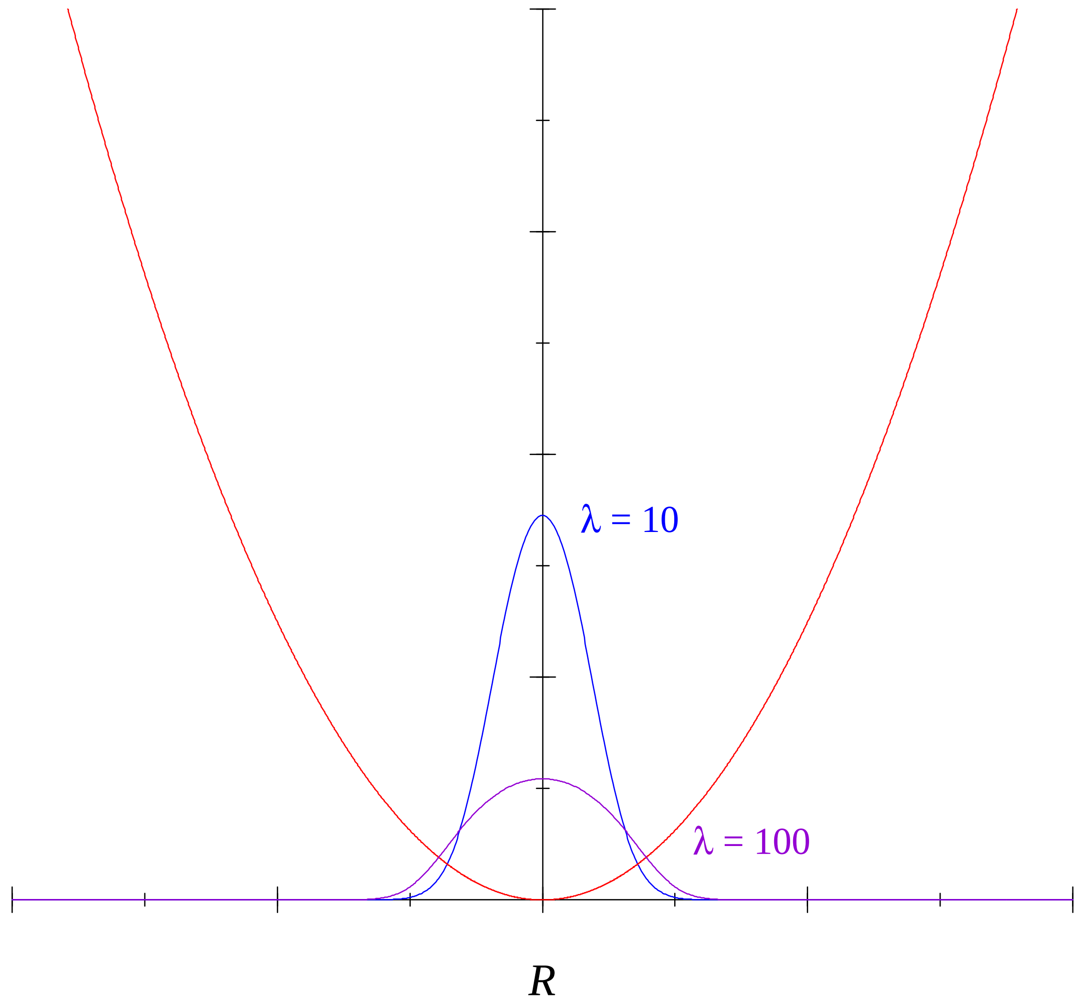

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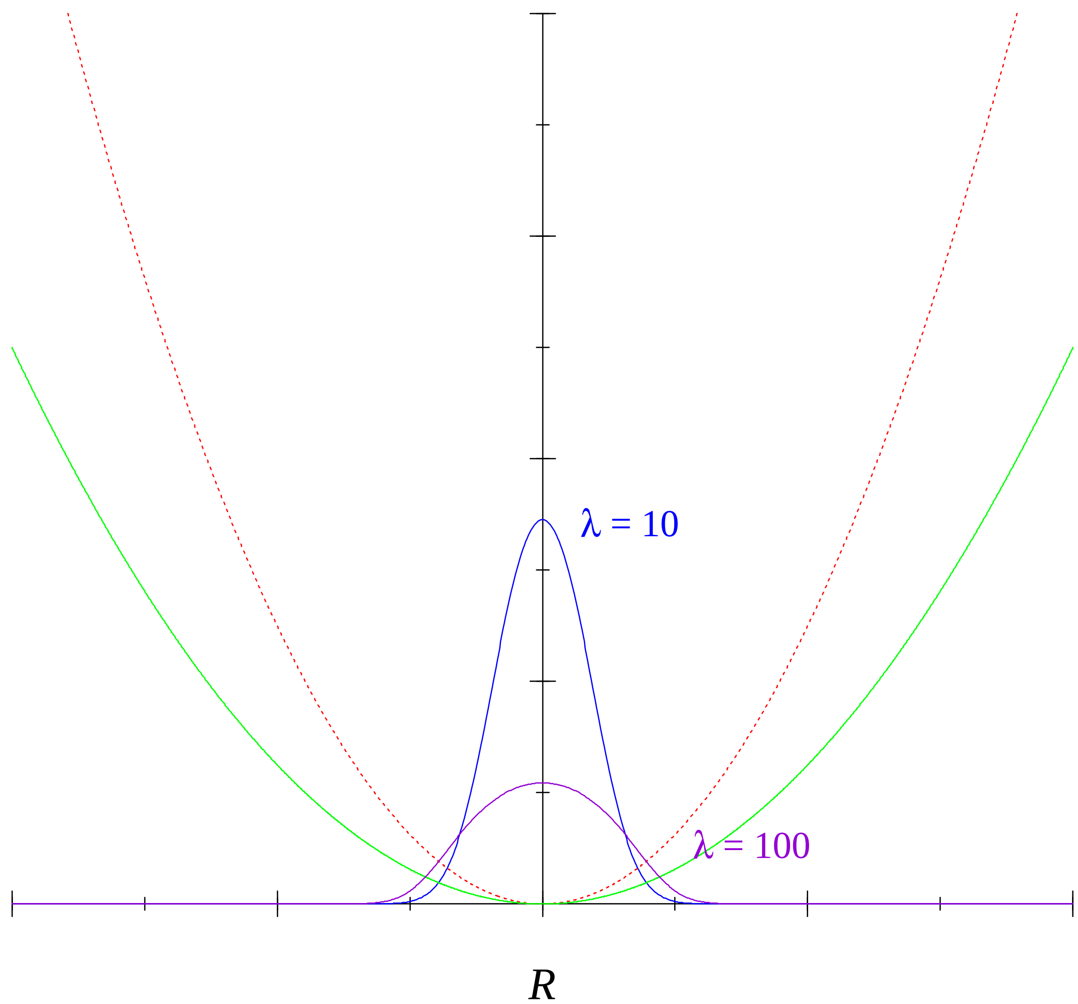

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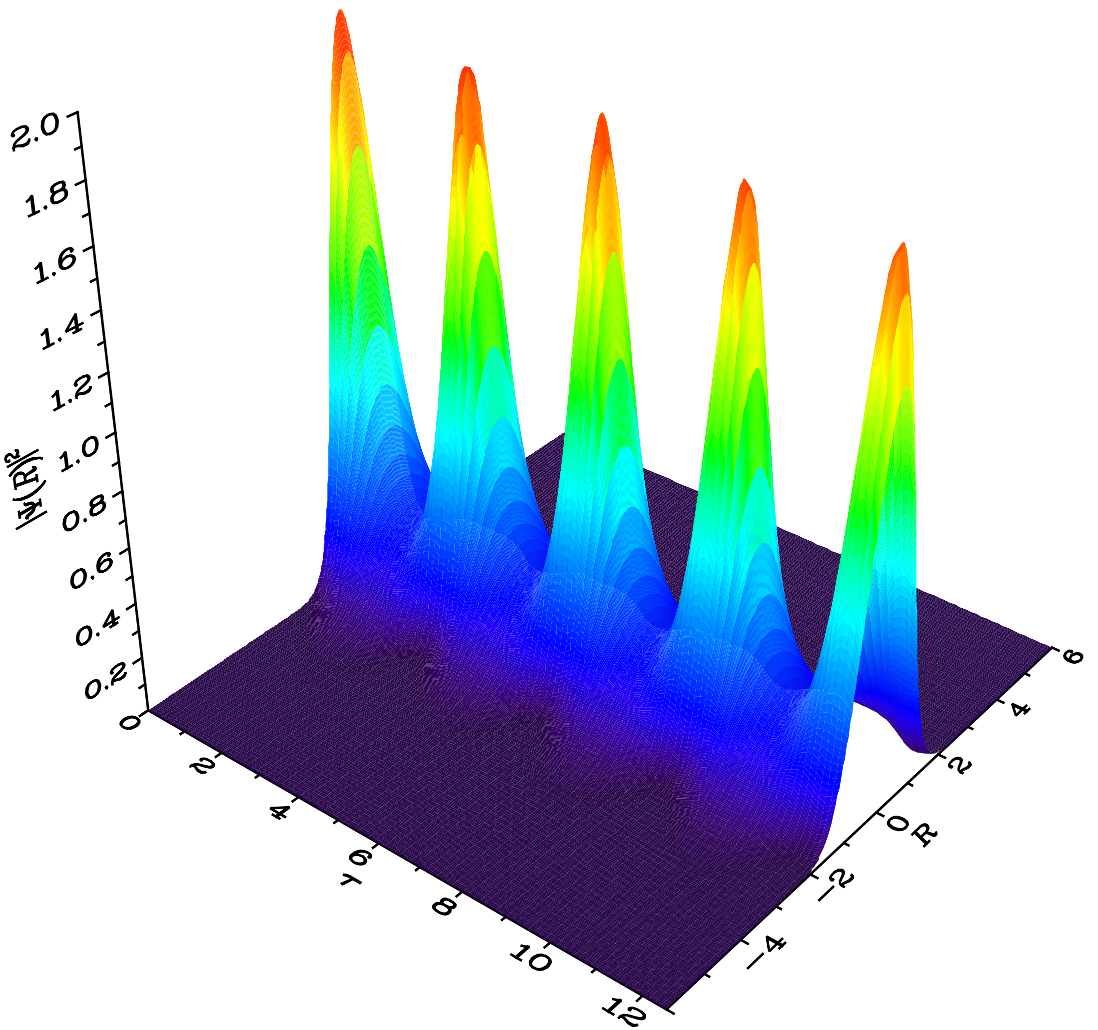
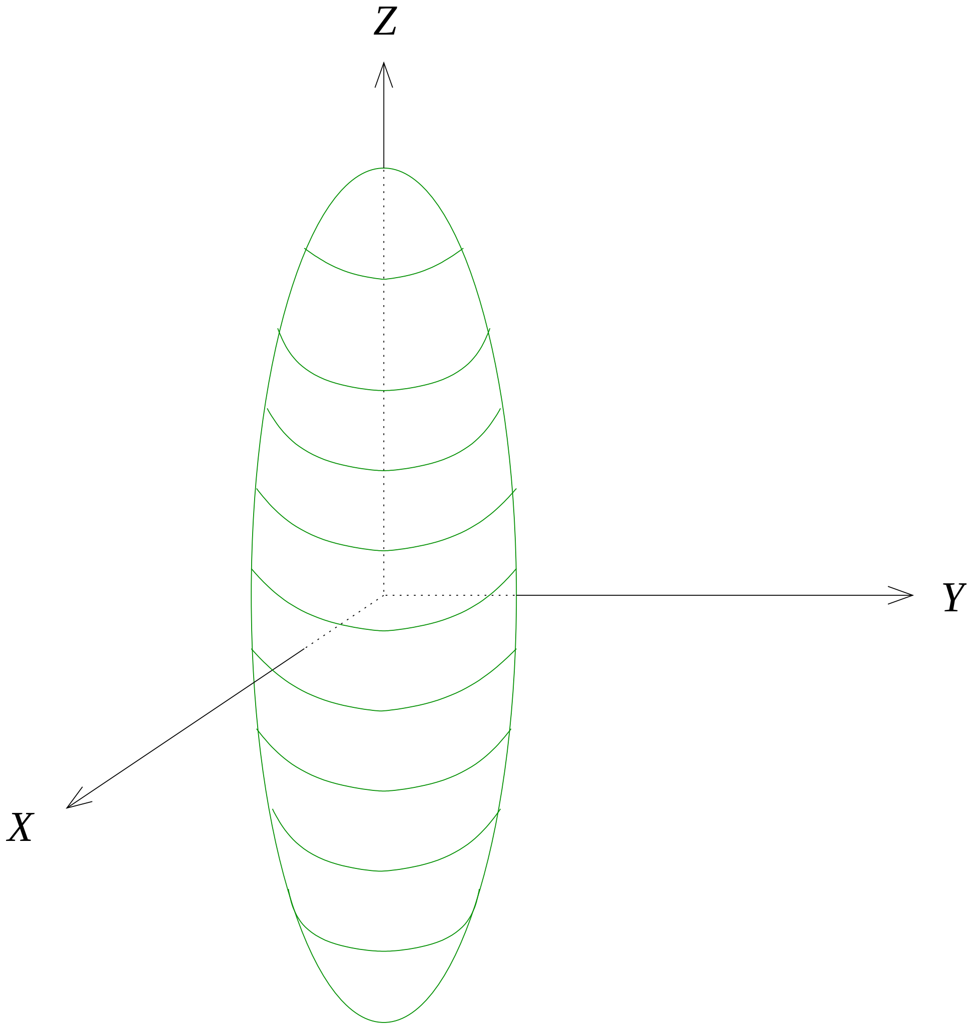
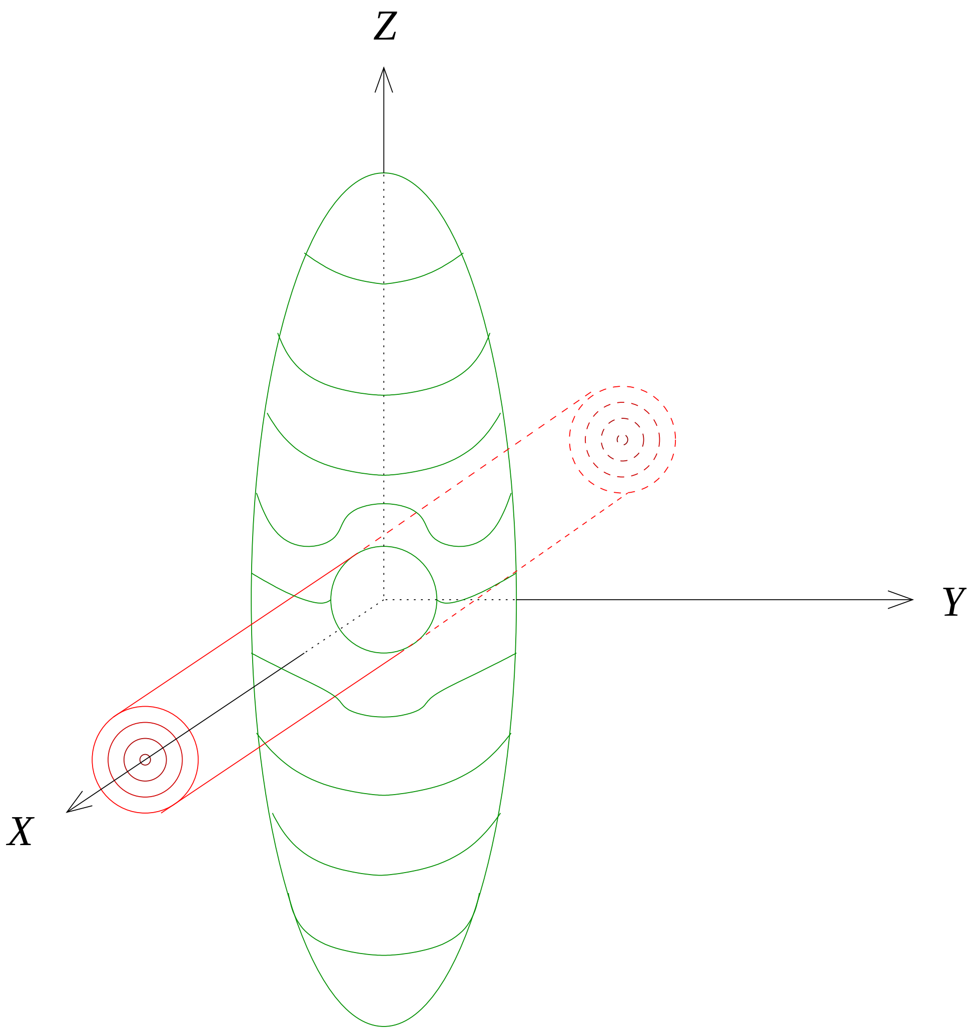


3D Example



3D Example



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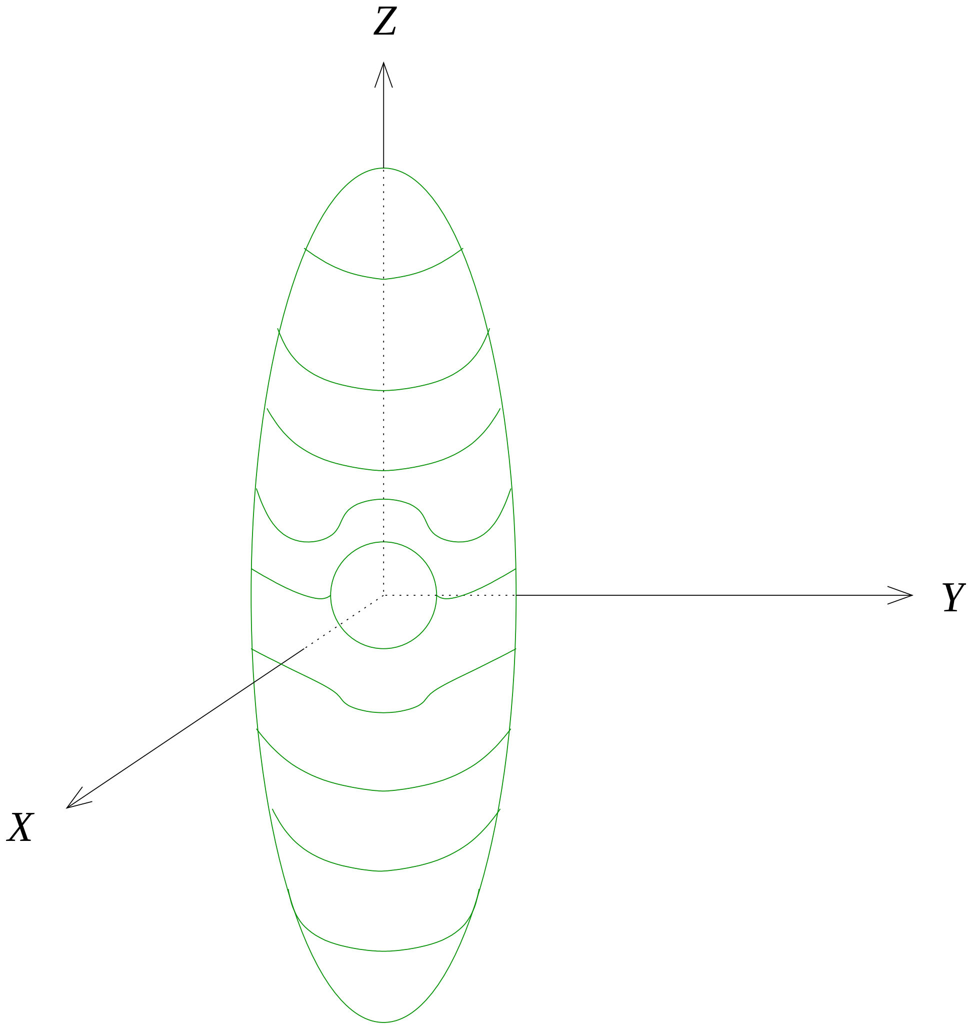
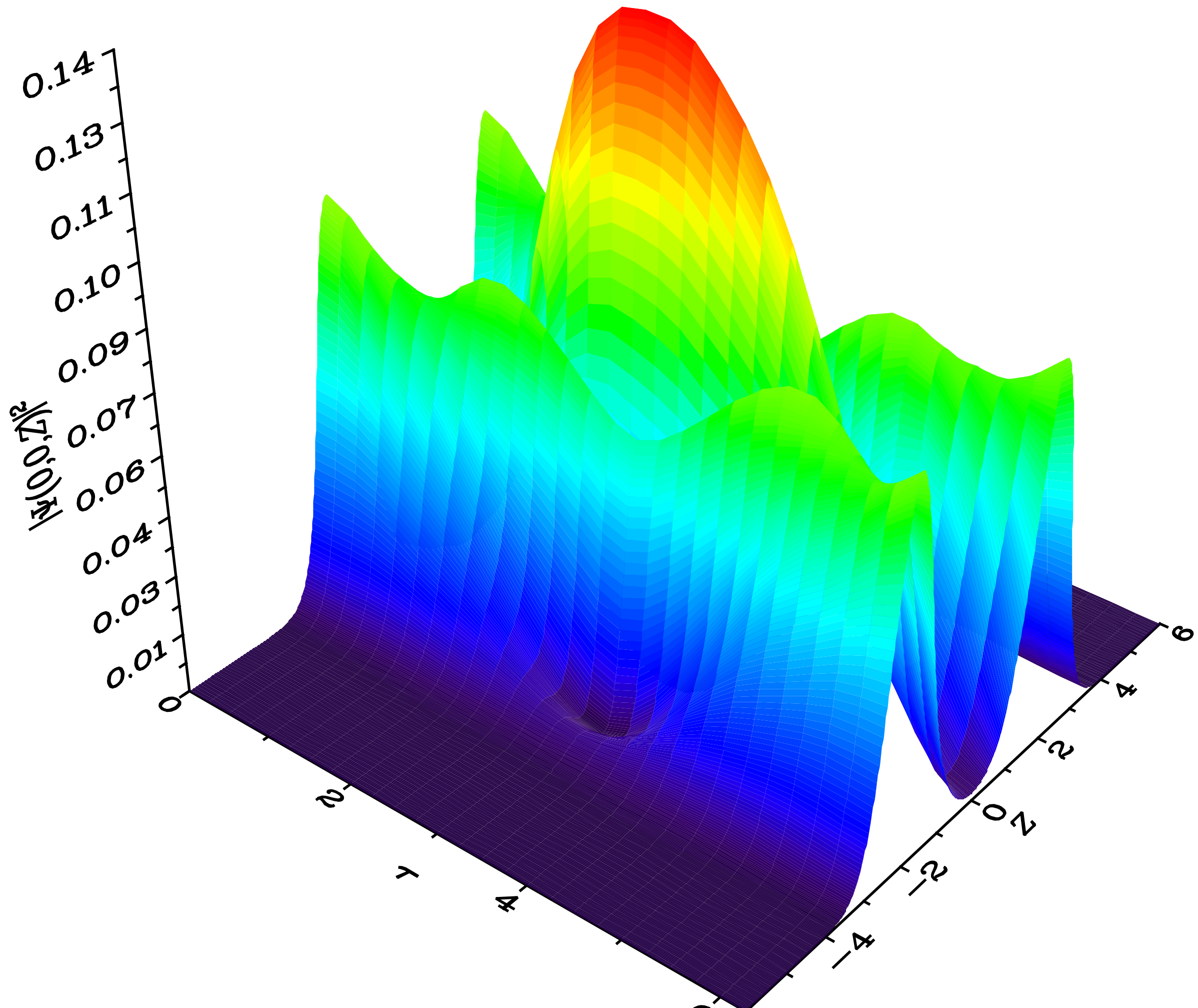


3D Example



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- Spectral method is used to solve the Gross-Pitaevskii equation
- Gauss-Hermite quadrature leads to an efficient algorithm
- Ground stationary state is obtained with the Optimal Damping Algorithm
- We can observe the time evolution of the condensate wave function

Perspectives

- Improved integration method

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  - Runge-Kutta with adaptive stepsize

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  - Runge-Kutta with adaptive stepsize
  - symplectic algorithms

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- Parallelized algorithm

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- Parallelized algorithm
- Treat coupled equations
  i.e., photoassociation in BECs:

$$
\begin{aligned}
i\hbar\frac{\partial\psi}{\partial t} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\rm a} + \lambda_{\rm aa}\left|\psi\right|^2 + \lambda_{\rm am}\left|\phi\right|^2\right]\psi + \alpha\phi\psi^* \\
i\hbar\frac{\partial\phi}{\partial t} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\rm m} + \lambda_{\rm mm}\left|\phi\right|^2 + \lambda_{\rm am}\left|\psi\right|^2\right]\phi + \tilde{\alpha}\psi^2
\end{aligned}
$$

Perspectives

- Improved integration method
- Parallelized algorithm
- Treat coupled equations
- Do some physics!

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Number of basis functions