Numerical simulation of the dynamics of the rotating dipolar Bose-Einstein condensates

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Outline

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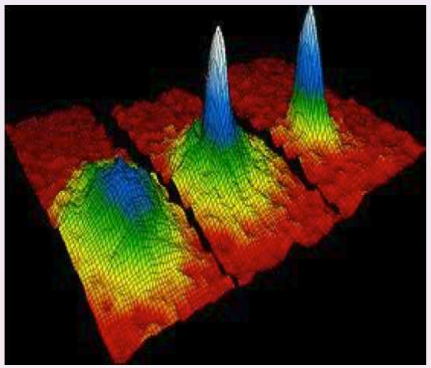
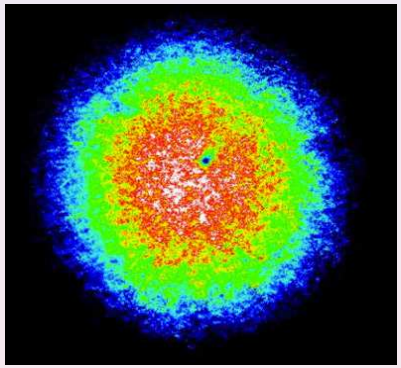
BEC

- Bose-Einstein condensate (BEC): many bosons occupy same quantum state if $T < T_c$.

  - Prediction: Einstein 1924
  - Experiments: JILA, BEC (1995), quantized vortex (1999)
  - Interaction between particles: short-range s-wave contact interaction





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[2] Shuman, Barry & Demile, Nature 467 (2010)

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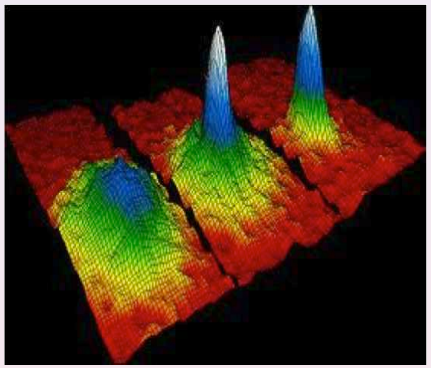

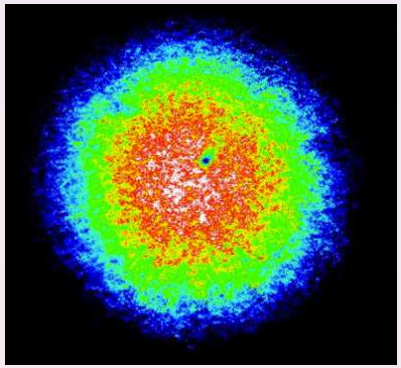

- Realization of BECs of ^{52}Cr (Chromium-52)[1] and creation of ultracold molecules[2]: long-range dipole-dipole interaction (DDI) between particle besides the contact interaction

  $\longrightarrow$ leading to fascinating and sometimes completely unexpected effects.

[1] Griesmaier, Werner, Hensler, Stuhler & Pfau, PRL 94 (2005)

[2] Shuman, Barry & Demile, Nature 467 (2010)

- Collapse even if the contact interaction are repulsive, dipole orientation $(0, 0, 1)$:

- Tunability of the dipole: dipole orientation $(\cos(0.2t), 0, \sin(0.2t))$

Gross-Pitaevskii equation (GPE): S. Yi and H. Pu, PRA 73 (2006); O'Dell, et al., PRA 80 (2009)

$$i\partial_t \psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta\,|\psi|^2 + \lambda\,\Phi(\mathbf{x},t) - \Omega\,L_z\right]\psi(\mathbf{x},t), \quad \mathbf{x}\in\mathbb{R}^d. \tag{1}$$

- $d = 2, 3$; $V(\mathbf{x})$: trapping potential; $L_z = -i(x\partial_y - y\partial_x) = -i\partial_\theta$.

[3] O'Dell et al., PRL 92 (2004); Bao et al., PRA 82 (2010)

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- $d = 2, 3$; $V(\mathbf{x})$: trapping potential; $L_z = -i(x\partial_y - y\partial_x) = -i\partial_\theta$.
- $\Phi(\mathbf{x},t)$: dipole-dipole interaction (DDI) potential, reads as[3]

$$\Phi(\mathbf{x},t) = U^d_{\rm dip} * |\psi|^2, \tag{2}$$

with

$$U^d_{\rm dip}(\mathbf{x},t) = \begin{cases} -\delta(\mathbf{x}) - 3\,\partial_{\mathbf{nn}}\left(\frac{1}{4\pi|\mathbf{x}|}\right), & d=3,\\ -\frac{3}{2}\left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\nabla_\perp^2\right)\left(\frac{1}{2\pi|\mathbf{x}|}\right), & d=2, \end{cases} \tag{3}$$

where $\mathbf{n} = (n_1(t), n_2(t), n_3(t))$, is the time (in)-dependent dipole axis, $\mathbf{n}_\perp = (n_1(t), n_2(t))$.

[3] O'Dell et al., PRL 92 (2004); Bao et al., PRA 82 (2010)

- Numerics: $\Omega = \lambda = 0$, time-splitting spectral method(TSSP)[4]

$$\text{Step 1}: i\partial_t \psi(\mathbf{x}, t) = -\frac{1}{2}\nabla^2 \psi(\mathbf{x}, t), \qquad \text{Step 2}: i\partial_t \psi(\mathbf{x}, t) = \left(V(\mathbf{x}) + \beta|\psi|^2\right)\psi(\mathbf{x}, t). \quad (4)$$

  - Step 1: discretised by spectral method and integrated in space exactly.
  - Step 2: nonlinear ODE solved analytically
  - Spectral in space, easy to implement.

[4] Bao, Jaksch & Markowich, JCP 03; Bao, Jin, Markowich, SIAM J. Sci. Comput., 03; etc

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  Cannot be simply extended to rotating system: $\Omega \neq 0$.

- Numerical difficulties: $\Omega \neq 0, \quad \lambda \neq 0$

  (1). rotating term: $L_z\psi$.

  (2). nonlocal DDI term: $\Phi(\mathbf{x},t) =: U_{\text{dip}}^d * |\psi|^2$.

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Outline

Consider only the rotational term first: i.e., $\lambda = 0$, $\Omega \neq 0$

$$L_z\psi(\mathbf{x}, t) = i(y\partial_x - x\partial_y)\psi(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^d, t \geq 0$$

Existing numerical methods: $\Omega \neq 0$, $\lambda = 0$, $L_z = i(y\partial_x - x\partial_y) = -i\partial_\theta$

- Time splitting + ADI: Bao and Wang, JCP, 2006.
- Time splitting + polar/cylindrical coordinates: Bao, Du and Zhang, SIAM J. Appl. Math., 2006.
- Time splitting + Laguerre-Fourier-Hermite: Bao, Li and Shen, SIAM J. Sci. Comupt., 2009.:

Existing numerical methods: $\Omega \neq 0,\ \lambda = 0,\ L_z = i(y\partial_x - x\partial_y) = -i\partial_\theta$

- Time splitting + ADI: Bao and Wang, JCP, 2006.
  - extra error for the splitting, not trivial to extend to higher order (in time) scheme.

$$\text{Step } 1 : i\partial_t \psi(\mathbf{x}, t) = \left[-\frac{1}{2}\partial_{xx} - \frac{1}{4}\partial_{zz} - i\Omega\ y\partial_x \right] \psi(\mathbf{x}, t). \tag{5}$$

$$\text{Step } 2 : i\partial_t \psi(\mathbf{x}, t) = \left[-\frac{1}{2}\partial_{yy} - \frac{1}{4}\partial_{zz} + i\Omega\ x\partial_y \right] \psi(\mathbf{x}, t). \tag{6}$$

$$\text{Step } 3 : i\partial_t \psi(\mathbf{x}, t) = \left[V(\mathbf{x}) + \beta|\psi|^2 \right] \psi(\mathbf{x}, t). \tag{7}$$

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- Time splitting + ADI: Bao and Wang, JCP, 2006.

- Time splitting + polar/cylindrical coordinates: Bao, Du and Zhang, SIAM J. Appl. Math., 2006.
  - only 2nd or 4th order accuracy in radial direction.

$$\text{Step } 1 : i\partial_t \psi(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 - \Omega L_z \right] \psi(\mathbf{x}, t). \tag{8}$$

$$\text{Step } 2 : i\partial_t \psi(\mathbf{x}, t) = \left[V(\mathbf{x}) + \beta |\psi|^2 \right] \psi(\mathbf{x}, t). \tag{9}$$

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- Time splitting + Laguerre-Fourier-Hermite: Bao, Li and Shen, SIAM J. Sci. Comupt., 2009.:
  - implementation of the code is quite involved.

$$\text{Step } 1 : i\partial_t \psi(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 - \Omega L_z + \frac{|\mathbf{x}|^2}{2} \right] \psi(\mathbf{x}, t). \tag{10}$$

$$\text{Step } 2 : i\partial_t \psi(\mathbf{x}, t) = \left[U(\mathbf{x}) + \beta |\psi|^2 \right] \psi(\mathbf{x}, t). \tag{11}$$

A rotating Lagrangian coordinate transformation

- Our method[5]: rotating Lagrangian coordinates transformation $\Longrightarrow$ relax ΩL_z $\Longrightarrow$ TSSP.

[5] Bao, Marahrens, Tang & Zhang, SIAM J. Sci. Comput., 13; Ming, Tang, & Zhang, J. Comput. Phys., 13

A rotating Lagrangian coordinate transformation

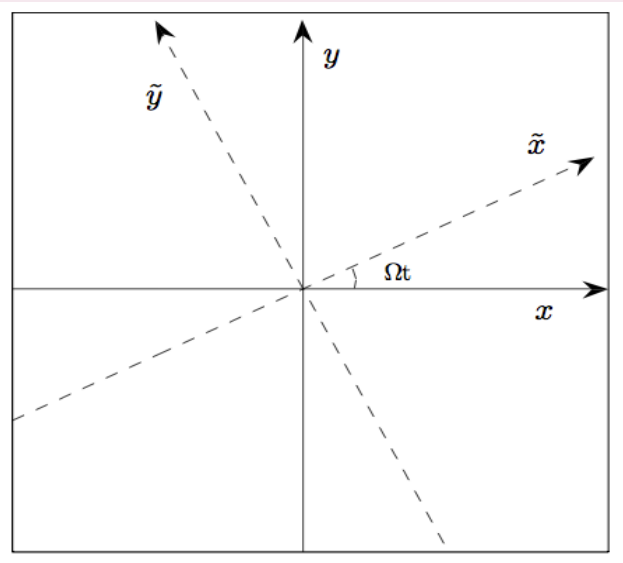
- Our method[5]: rotating Lagrangian coordinates transformation $\Longrightarrow$ relax ΩL_z $\Longrightarrow$ TSSP.
- Rotating Lagrangian coordinates $\widetilde{\mathbf{x}}$:

$$\widetilde{\mathbf{x}} = \mathbf{A}^{-1}(t)\mathbf{x} = \mathbf{A}^{T}(t)\mathbf{x} \quad \Leftrightarrow \quad \mathbf{x} = \mathbf{A}(t)\widetilde{\mathbf{x}}, \qquad \mathbf{x} \in \mathbb{R}^d. \tag{12}$$

where $\mathbf{A}(t)$: orthogonal rotational matrix defined in 3-d,respectively, 2-d

$$\mathbf{A}(t) = \begin{pmatrix} \cos(\Omega t) & \sin(\Omega t) & 0 \\ -\sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{A}(t) = \begin{pmatrix} \cos(\Omega t) & \sin(\Omega t) \\ -\sin(\Omega t) & \cos(\Omega t) \end{pmatrix}. \tag{13}$$

- Geometrical relation: Cartesian vs rotating Lagrangian coordinates.



[5] Bao, Marahrens, Tang & Zhang, SIAM J. Sci. Comput., 13; Ming, Tang, & Zhang, J. Comput. Phys., 13

New formation of GPE, simple and efficient numerical method

- (Recall) GPE in Cartesian coordinate:

$$i\partial_t \psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\psi|^2\right]\psi(\mathbf{x},t) - \Omega L_z \psi(\mathbf{x},t). \tag{14}$$

- Take rotating Lagrangian transformation, set $\phi(\widetilde{\mathbf{x}},t) := \psi(\mathbf{x},t) = \psi\left(\mathbf{A}(t)\widetilde{\mathbf{x}},t\right)$,
- GPE with rotational term in rotating Lagrangian coordinate

$$i\partial_t \phi(\widetilde{\mathbf{x}},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{A}(t)\widetilde{x}) + \beta|\phi|^2\right]\phi(\widetilde{\mathbf{x}},t). \tag{15}$$

- TSSP methods:

$$\text{Step 1}: \quad i\partial_t \phi(\widetilde{\mathbf{x}},t) = -\frac{1}{2}\nabla^2 \phi(\widetilde{\mathbf{x}},t). \tag{16}$$

$$\text{Step 2}: \quad i\partial_t \phi(\widetilde{\mathbf{x}},t) = \left(V(\mathbf{A}(t)\widetilde{x}) + \beta|\phi|^2\right)\phi(\widetilde{\mathbf{x}},t). \tag{17}$$

Taking back the nonlocal dipolar term

- Reformulate GPE and truncated into bounded domain problem, $\mathcal{D} \subset \mathbb{R}^d$ bounded:

$$i\partial_t \phi(\widetilde{\mathbf{x}}, t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{A}(t)\widetilde{x}) + \beta|\phi|^2 + \lambda\, \widetilde{U}^d_{\mathrm{dip}} * |\phi(\widetilde{\mathbf{x}}, t)|^2 \right] \phi(\widetilde{\mathbf{x}}, t), \qquad \widetilde{\mathbf{x}} \in \overline{\mathcal{D}} \tag{18}$$

$$\text{with} \quad \widetilde{U}^d_{\mathrm{dip}}(\widetilde{\mathbf{x}}, t) = \begin{cases} -\delta(\widetilde{\mathbf{x}}) - 3\partial_{\mathbf{mm}} \left(\frac{1}{4\pi|\widetilde{\mathbf{x}}|} \right), & \mathbf{m}(t) = \mathbf{A}(t)\mathbf{n}(t), \quad d = 3, \\ -\frac{3}{2} \left(\partial_{\mathbf{m}_\perp \mathbf{m}_\perp} - m_3^2 \nabla_\perp^2 \right) \left(\frac{1}{2\pi|\widetilde{\mathbf{x}}|} \right), & \mathbf{m}_\perp(t) = \mathbf{A}(t)\mathbf{n}_\perp(t), \quad d = 2, \end{cases} \tag{19}$$

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- TSSP methods: for $t_n < t < t_{n+1}$

$$\text{Step 1}: \quad i\partial_t \phi(\widetilde{\mathbf{x}}, t) = -\frac{1}{2}\nabla^2 \phi(\widetilde{\mathbf{x}}, t) \tag{20}$$

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Step 2: $\rightarrow$ density $\rho(\mathbf{x}, t) =: |\phi(\widetilde{\mathbf{x}}, t)|^2 = |\phi(\widetilde{\mathbf{x}}, t_n)|^2 =: \rho^n(\widetilde{\mathbf{x}}) \rightarrow$ integrate analytically

$$\phi(\widetilde{\mathbf{x}}, t) = \exp\left\{ -i \left[\beta \rho^n(\widetilde{\mathbf{x}})(t - t_n) + \int_{t_n}^{t} \left(V(A(\tau)\widetilde{\mathbf{x}}) + \widetilde{U}^d_{\rm dip}(\widetilde{\mathbf{x}}, \tau) * \rho^n(\widetilde{\mathbf{x}}) \right) d\tau \right] \right\} \tag{22}$$

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- Reformulate GPE and truncated into bounded domain problem, $\mathcal{D} \subset \mathbb{R}^d$ bounded:

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Question: How to evaluate the nonlocal DDI term: $\widetilde{\Phi} = \widetilde{U}^d_{\rm dip} * \rho^n(\widetilde{\mathbf{x}})$?

Evaluation of nonlocal potential:

$$\widetilde{\Phi} = \widetilde{U}^{d}_{\mathrm{dip}} * \rho^{n}(\widetilde{\mathbf{x}})$$

Numerical methods to evaluate the nonlocal term

Nonlocal DDI potential

$$\widetilde{\Phi} = \widetilde{U}^d_{\rm dip} * \rho^n(\widetilde{\mathbf{x}}) \tag{23}$$

with

$$\widetilde{U}^d_{\rm dip} = \begin{cases} -\delta(\widetilde{\mathbf{x}}) - 3\,\partial_{\mathbf{mm}}\left(\frac{1}{4\pi|\widetilde{\mathbf{x}}|}\right), \\ -\frac{3}{2}\left(\partial_{\mathbf{m}_\perp\mathbf{m}_\perp} - n_3^2\nabla_\perp^2\right)\left(\frac{1}{2\pi|\widetilde{\mathbf{x}}|}\right), \end{cases} \Longleftrightarrow \widehat{\widetilde{U}}^d_{\rm dip} = \begin{cases} -1 + \frac{3(\mathbf{m}\cdot\mathbf{k})^2}{\|\mathbf{k}\|^2}, & d=3, \\ \frac{3\left[(\mathbf{m}_\perp\cdot\mathbf{k})^2 - m_3^2\|\mathbf{k}\|^2\right]}{2\|\mathbf{k}\|}, & d=2, \end{cases} \tag{24}$$

where $\widehat{\widetilde{U}}^d_{\rm dip}(\mathbf{k},t) =: \mathcal{F}\left\{\widetilde{U}^d_{\rm dip}(\widetilde{\mathbf{x}},t)\right\}$ denotes the Fourier transform of $\widetilde{U}^d_{\rm dip}$

- Naturally, convolution theorem + standard fast Fourier transform (FFT)[6]

$$\widetilde{\Phi}(\widetilde{\mathbf{x}},t) = \mathcal{F}^{-1}\left\{\widehat{\rho^n}\,\widehat{\widetilde{U}}^d_{\rm dip}\right\} \tag{25}$$

  - standard FFT: uniform grid points in Cartesian coordinates, require value of 0-mode in Fourier space
  - singularity of $\widehat{\widetilde{U}}^d_{\rm dip}(\mathbf{k},t)$ at $\mathbf{k}=0 \Longrightarrow$ locking phenomena

[6] Lahaye, Metz, Fröhlich, Koch, Meister, Griesmaier, Pfau, Saito, Kawaguchi & Ueda, Phys. Rev. Lett., 08

Numerical methods to evaluate the nonlocal term: $\widetilde{\Phi} = \widetilde{U}^d_{\rm dip} * \rho^n(\widetilde{\mathbf{x}})$

- Avoid the use of 0-mode: reformulate problem to equivalent poisson/fractional-poisson[7]:

$$\widehat{\widetilde{U}}^d_{\rm dip} = \begin{cases} -\delta(\widetilde{\mathbf{x}}) - 3\partial_{\mathbf{mm}}\left(\frac{1}{4\pi|\widetilde{\mathbf{x}}|}\right), \\ -\frac{3}{2}\left(\partial_{\mathbf{m}_\perp\mathbf{m}_\perp} - m_3^2\nabla_\perp^2\right)\left(\frac{1}{2\pi|\widetilde{\mathbf{x}}|}\right), \end{cases} \Rightarrow \widetilde{\Phi}(\widetilde{\mathbf{x}},t) = \begin{cases} -\rho^n(\widetilde{\mathbf{x}}) + 3\partial_{\mathbf{mm}}\varphi, \\ \frac{3}{2}\left(\partial_{\mathbf{m}_\perp\mathbf{m}_\perp} - m_3^2\nabla_\perp^2\right)\varphi, \end{cases} \tag{26}$$

with

$$\left.\begin{array}{ll} d=3: & -\Delta \\ d=2: & \sqrt{-\Delta} \end{array}\right\} \varphi(\widetilde{\mathbf{x}},t) = \rho^n(\widetilde{\mathbf{x}}) \quad \text{with} \quad \lim_{|\widetilde{\mathbf{x}}|\to\infty} \varphi(\widetilde{\mathbf{x}},t) = 0. \tag{27}$$

  - homogeneous Dirichlet BC + discrete sine spectral (DST)
  - Polynomial decay of $\varphi(\widetilde{\mathbf{x}},t) \longrightarrow$ large computational domain to reduce the boundary truncation error:

[7] Bao, Cai, & Wang, J. Comput. Phys., 10; Bao, Marahrens, Tang & Zhang, SIAM J. Sci. Comput., 13;

Numerical methods to evaluate the nonlocal term: $\widetilde{\Phi} = \widetilde{U}^d_{\rm dip} * \rho^n(\widetilde{\mathbf{x}})$

- For example, we take $d = 3$, and

$$\rho^n(\widetilde{\mathbf{x}}) = e^{-|\widetilde{\mathbf{x}}|^2/c^2} \Longrightarrow \quad \widetilde{\Phi} = -\rho^n(\widetilde{\mathbf{x}}) - 3\,\mathbf{m}^T\mathbf{D}\,\mathbf{m} \tag{28}$$

here, the Hessian matrix $\mathbf{D}$ is given as follows:

$$\begin{aligned}\mathbf{D}_{ij} \quad = \quad & \delta_{ij}\Big(\frac{c^2}{2|\widetilde{\mathbf{x}}|^2}e^{-\frac{|\widetilde{\mathbf{x}}|^2}{c^2}} - \frac{c^3\sqrt{\pi}}{4|\widetilde{\mathbf{x}}|^3}\mathrm{Erf}\Big(\frac{|\widetilde{\mathbf{x}}|}{c}\Big)\Big) \\ & + \mathbf{x}_i\mathbf{x}_j\Big(-\frac{3\,c^2}{2\,|\widetilde{\mathbf{x}}|^4}e^{-\frac{|\widetilde{\mathbf{x}}|^2}{c^2}} - \frac{1}{|\widetilde{\mathbf{x}}|^2}e^{-\frac{|\widetilde{\mathbf{x}}|^2}{c^2}} + \frac{3\,c^3\sqrt{\pi}}{4\,|\widetilde{\mathbf{x}}|^5}\mathrm{Erf}\Big(\frac{|\widetilde{\mathbf{x}}|}{c}\Big)\Big).\end{aligned}$$

where δ_{ij} is the dirac function and $\mathrm{Erf}(r)$ is the error function defined as $\mathrm{Erf}(r) = \frac{2}{\sqrt{\pi}}\int_0^r e^{-t^2}\,dt$.

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- Let $\mathbf{m} = (0,0,1)^T$, $c = 1.4$, solve $\widetilde{\Phi}$ on computational domain $\mathcal{D} = [-L, L]^3$ with h the mesh size via DST and compare with the exact solution (28).

Table: l^2-errors of $\widetilde{\Phi}$ by DST on $\mathcal{D}[-L, L]^2$.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	6.919E-02	7.720E-02	8.124E-02	8.327E-02
$L = 16$	2.709E-02	2.853E-02	2.925E-02	2.961E-02
$L = 32$	1.008E-02	1.033E-02	1.046E-02	1.052E-02

Numerical methods to evaluate the nonlocal term: $\widetilde{\Phi} = \widetilde{U}^d_{\rm dip} * \rho^n(\widetilde{\mathbf{x}})$

- Convolution theorem +coordinate transform +non-uniform fast Fourier transform (NUFFT)[8]

$$\widetilde{\Phi}(\widetilde{\mathbf{x}},t) = \mathcal{F}^{-1}\left\{\widehat{\rho^n}\,\widehat{\widetilde{U}}^d_{\rm dip}\right\}, \quad \text{with} \quad \widehat{U}^d_{\rm dip} = \begin{cases} \frac{3\left[(\mathbf{m}_\perp\cdot\mathbf{k})^2 - m_3^2\|\mathbf{k}\|^2\right]}{2\|\mathbf{k}\|}, & d=2 \\ -1+\frac{3(\mathbf{m}\cdot\mathbf{k})^2}{\|\mathbf{k}\|^2}, & d=3 \end{cases} \tag{29}$$

- Singularity at $\mathbf{k}=\mathbf{0}$ removable: adopt spherical/polar coordinate transform in 3-d/2-d

$$\widetilde{\Phi}(\widetilde{\mathbf{x}},t) = \int_{\mathbb{R}^d} \frac{e^{i\,\mathbf{k}\cdot\widetilde{\mathbf{x}}}\widehat{U}^d_{\rm dip}(k,t)\,\widehat{\rho^n}(\mathbf{k})}{(2\pi)^d}\,d\mathbf{k} \approx \int_{\|\mathbf{k}\|<R} \frac{e^{i\,\mathbf{k}\cdot\mathbf{x}}\widehat{U}^d_{\rm dip}(k,t)\,\widehat{\rho^n}(\mathbf{k})}{(2\pi)^d}\,d\mathbf{k}$$

$$= \begin{cases} \frac{1}{4\pi^2}\int_0^R\int_0^{2\pi} e^{i\,\mathbf{k}\cdot\mathbf{x}}\,\|\mathbf{k}\|\,\widehat{U}^d_{\rm dip}\,\widehat{\rho^n}\,dr\,d\phi, & d=2 \\ \frac{1}{8\pi^3}\int_0^R\int_0^{\pi}\int_0^{2\pi} e^{i\,\mathbf{k}\cdot\mathbf{x}}\,\|\mathbf{k}\|^2\,\widehat{U}^d_{\rm dip}\,\widehat{\rho^n}\,\sin\theta\,dr\,d\theta\,d\phi, & d=3 \end{cases} \tag{30}$$

- Further discretized by high-order Gauss quadrature:
  - Azimuthal ϕ-direction: trapezoidal rule
  - radial r-direction (and inclination θ-direction in 3d): (shifted and scaled) Gauss-Legendre quadrature

[8] Bao, Greengard & Jiang, SIAM J. Sci. Comput., 2014, Bao, Tang & Zhang, preprint, 2014

NUFFT to evaluate the nonlocal term: $\widetilde{\Phi} = \widetilde{U}^d_{\text{dip}} * \rho^n(\widetilde{\mathbf{x}})$

- Same example as the DST one, now we solve $\widetilde{\Phi}$ by NUFFT.

Table: l^2-errors of $\widetilde{\Phi}$ by NUFFT on $\mathcal{D}[-L, L]^2$.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	3.428E-4	9.834E-12	1.601E-14	<1E-14
$L = 16$	3.551E-4	1.143E-11	8.089E-15	<1E-15

Extension to rotating two-component dipolar BEC

Extension to rotating two-component dipolar BEC[9]

Rotating two-component GPE: $j = 1, 2$

$$i\partial_t \psi_j(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 + V_j(\mathbf{x}) - \Omega \mathrm{L}_z + \sum_{l=1}^{2} (\beta_{jl}|\psi_l|^2 + \lambda_{jl}\Phi_l) \right] \psi_j(\mathbf{x}, t) - \kappa \psi_{3-j}, \quad (31)$$

$$\Phi_l(\mathbf{x}, t) = U_{\mathrm{dip}}^d * |\psi_l(\mathbf{x}, t)|^2, \qquad l = 1,\ 2, \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0 \quad (32)$$

- κ: Rabi frequency represents the internal atomic Josephson Junction effect (JJE).

[9] Saito, Kawaguchi and Ueda, PRL 102 (2009), Ming, Tang & Zhang, JCP 258 (2013), Bao, Mauser, Tang & Yong, preprint, 2014

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- κ: Rabi frequency represents the internal atomic Josephson Junction effect (JJE).
- Take rotating Lagrangian transformation: $\phi_j(\widetilde{\mathbf{x}}, t) := \psi(\mathbf{A}(t)\mathbf{x})$

$$i\frac{\partial \phi_j(\widetilde{\mathbf{x}}, t)}{\partial t} = \left[-\frac{1}{2}\nabla^2 + V_j(\mathbf{A}(t)\widetilde{\mathbf{x}}, t) + \sum_{l=1}^{2} \left(\beta_{jl}|\phi_l|^2 + \lambda_{jl}\widetilde{\Phi}_j\right) \right] \phi_j - \kappa \phi_{3-j}(\widetilde{\mathbf{x}}, t), \quad (33)$$

$$\widetilde{\Phi}_l(\mathbf{x}, t) = \widetilde{U}_{\mathrm{dip}}^d * |\phi_l(\widetilde{\mathbf{x}}, t)|^2, \qquad l = 1,\ 2, \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0 \quad (34)$$

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Extension to rotating two-component BEC

- TSSP methods:

$$\text{Step 1}: \quad i\partial_t \phi_j(\widetilde{\mathbf{x}}, t) = \left(V_j(\mathbf{A}(t)\widetilde{\mathbf{x}}, t) + \sum_{l=1}^{2} (\beta_{jl}|\phi_l|^2 + \lambda_{jl}\widetilde{\Phi}_j) \right) \phi_j \tag{35}$$

$$\text{Step 2}: \quad i\partial_t \phi_j(\widetilde{\mathbf{x}}, t) = -\frac{1}{2}\nabla^2 \phi_j(\widetilde{\mathbf{x}}, t) - \kappa\psi_{3-j} \tag{36}$$

- Step 2: set $\varphi_1(\widetilde{\mathbf{x}}, t) = \phi_1 + \phi_2$ and $\varphi_2(\widetilde{\mathbf{x}}, t) = \phi_1 - \phi_2 \Leftrightarrow \phi_1 = \frac{\varphi_1+\varphi_2}{2}$ and $\phi_2 = \frac{\varphi_1-\varphi_2}{2}$

$$i\partial_t \varphi_1(\widetilde{\mathbf{x}}, t) = -\frac{1}{2}\nabla^2 \varphi_1(\widetilde{\mathbf{x}}, t) - \kappa\varphi_1, \tag{37}$$

$$i\partial_t \varphi_2(\widetilde{\mathbf{x}}, t) = -\frac{1}{2}\nabla^2 \varphi_2(\widetilde{\mathbf{x}}, t) + \kappa\varphi_2 \tag{38}$$

Outline

Test of accuracy: one-component BEC

- Let $d = 3$, dipole axis $\mathbf{n} = \mathbf{m} = (0, 0, 1)^T$, computational domain $\mathcal{D} = [-8, 8]^3$, let initial data be

$$\psi^0(\mathbf{x}) = \frac{1}{\pi^{3/4}} e^{-(x^2+y^2+z^2)/2}, \tag{39}$$

and take $\gamma_x = \gamma_y = \gamma_z = 1$, $\Omega = 0$. We compute the exact solution at time $t = 0.28$ with very small mesh size $h = \frac{1}{16}$ and $\tau = 0.0001$, and $\lambda = \frac{\beta}{2}$.

Table: l^2-error at $t = 0.28$ in spatial direction (upper parts) and temporal direction (lower parts

	$h = 1/2$	$1/4$	$1/8$	$1/16$
$\beta = 2$	3.999E-3	1.612E-5	1.601E-11	3.049E-12
$\beta = 10$	1.773E-2	2.581E-4	8.899E-9	3.133E-12
$\beta = 50$	8.074E-2	8.186E-3	2.460E-5	2.304E-11
	$\tau = 0.008$	$\tau/2$	$\tau/4$	$\tau/8$
$\beta = 2$	2.983E-6	7.454E-7	1.860E-7	4.615E-8
$\beta = 10$	8.151E-6	2.036E-6	5.081E-7	1.261E-7
$\beta = 50$	8.427E-5	2.105E-5	5.251E-6	1.303E-6

Application to two-component dipolar BEC

- Initial data: ground state under parameters

$$\mathbf{n} = (0, 0, 1), \gamma_x = \gamma_y = \gamma_z = 1, \Omega = 0, \kappa = 0, \tag{40}$$

$$\beta_{12} = \beta_{21} = \lambda_{12} = \lambda_{21} = 0, \beta_{11} = \beta_{22} = 103.58, \lambda_{11} = \lambda_{22} = 82.864. \tag{41}$$

Dynamics: change parameters: $\beta_{12} = \beta_{21} = 100$ and $\lambda_{22} = 0$.

Outline

- Numerical methods on dynamic simulation of rotating dipolar BEC was presented:
  - Rotating Lagrangian Coordinate transformation to eliminate the constrain of rotation term
  - NUFFT to evaluate non-local DDI potential
- Easy to apply to other system: rotating multi-component BECs, rotating spin-orbit coupling BEC, etc...

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Thank You For Attention!