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Finite element methods for dipolar BEC

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Summary

GP equations for the dipolar BEC

In the ultracold gas, the dipole-dipole interaction (DDI)is long-range and anisotropic. The DDI between alkali atoms is a thousand times smaller than the short-range interaction. However, DDI between transition atoms is large (52Cr) [Pfau,PRL, 2005]. The dipolar BEC is governed by the 3D Gross-Pitaevskii equation (GPE). By the dimensionless transformation, one gets the following nonlocal GPE:

$$i\psi_t(\mathbf{x},\mathbf{t}) = (-\frac{\mathbf{1}}{\mathbf{2}}\nabla^2 + \mathbf{V}(\mathbf{x}) + \beta|\psi(\mathbf{x},\mathbf{t})|^2 + \lambda\,\mathbf{U_{dip}} * |\psi(\mathbf{x},\mathbf{t})|^2)\psi(\mathbf{x},\mathbf{t}) \quad (1)$$

where $V(\mathbf{x}) = \frac{1}{2}(\gamma_1^2x^2 + \gamma_2^2y^2 + \gamma_3^2z^2)$ and $U_{dip} = \frac{C_{dd}}{4\pi}\frac{1-3\cos^2\theta}{|\mathbf{x}|^3}$.

GP equations for the dipolar BEC

GPE has two conservation quantities, i.e, the number of the particles and the total energy:

$$\int_{\mathbb{R}^3} |\psi(\mathbf{x},t)|^2 d\mathbf{x} \equiv \int_{\mathbb{R}^3} |\psi(\mathbf{x},\mathbf{0})|^2 \mathbf{dx} = \int_{\mathbb{R}^3} |\psi_{\mathbf{0}}(\mathbf{x})|^2 \mathbf{dx} = \mathbf{1} \qquad (2)$$

and

$$\begin{aligned} E(\psi(\mathbf{x},\mathbf{t})) &= \int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta}{\mathbf{2}}|\psi|^4 + \frac{\lambda}{\mathbf{2}}(\mathbf{U_{dip}} * |\psi|^2)|\psi|^2 \right) \mathbf{dx} \\ &\equiv E(\psi(\mathbf{x},\mathbf{0})) \end{aligned} \qquad (3)$$

Some efficient numerical method: time-splitting spectral (Bao et.al. 2010; Bao, et.al,arXiv:1410.3584;Markowich et. al., 2014);Finite difference method;Finite element method。

Summary

FEM for the ground state of the 1D dipolar BEC

To obtain the ground state of the 1D dipolar BEC, we apply the imaginary time method, that is, solve the following equation and combine projection method:

$$\begin{aligned}\psi_t(x,t) &= \frac{1}{2}\nabla^2\psi - V(x)\psi(x,t) - \beta|\psi(x,t)|^2\psi(x,t) \\ &\quad -\lambda(U_{dip} * |\psi(x,t)|^2)\psi(x,t), -a < x < a \qquad (4)\end{aligned}$$

where $V(x) = \frac{x^2}{2}$, $U_{dip} = |x|^{-\alpha}$ with $0 < \alpha < 1$. The boundary condition is $\psi(-a,t) = \psi(a,t) = 0$; Initial condition is $\psi(x,0) = \psi_0(x)$

FEM for the ground state of the 1D dipolar BEC

FEM is to find the real function $\psi_h(x,t) = \sum_{i=0}^{m} \alpha_i(t)\phi_i(x) \in V_h(\Omega)$, which satisfies $\forall \phi(x) \in V_h(\Omega)$, $\Omega = [-a, a]$

$$\begin{cases} \int_\Omega \psi_{ht}\phi dx = \int_\Omega \left(\frac{1}{2}\nabla^2 - V(x) - \beta|\psi_h|^2 - \lambda(U_{dip} * |\psi_h|^2) \right)\psi_h\phi \, dx, \\ \int_\Omega \psi_h(x,0)\phi dx = \int_R \psi_0(x)\phi dx, \end{cases} \tag{5}$$

$$\sum_{i=0}^{m} \alpha_i'(t) \int_\Omega \phi_i(x)\phi_j(x)dx =$$

$$-\frac{1}{2}\sum_{i=0}^{m} \alpha_i(t) \int_\Omega \nabla\phi_i(x)\cdot\nabla\phi_j(x)dx - \sum_{i=0}^{m} \alpha_i(t) \int_\Omega V(x)\phi_i(x)\phi_j(x)dx$$

$$-\beta\sum_{i=0}^{m} \alpha_i(t) \int_\Omega |\sum_{k=0}^{m} \alpha_k(t)\phi_k(x)|^2\phi_i(x)\phi_j(x)dx$$

$$-\lambda\sum_{i=0}^{m} \alpha_i(t) \int_\Omega U_{dip} * (|\sum_{k=0}^{m} \alpha_k(t)\phi_k(x)|^2)\phi_i(x)\phi_j(x)dx, \quad 0 \le j \le m.$$

FEM for the ground state of the 1D dipolar BEC

Denote $A_{ij} = \int_\Omega \phi_i(x)\phi_j(x)dx$,
$B_{ij} = \int_\Omega \nabla\phi_i(x) \cdot \nabla\phi_j(x)dx$,
$C_{ij} = \int_\Omega V(x)\phi_i(x)\phi_j(x)dx$,
$D(\alpha)_{ij} = \int_\Omega |\sum_{k=0}^m \alpha_k(t)\phi_k(x)|^2\phi_i(x)\phi_j(x)dx$
$K(\alpha)_{ij} = \int_\Omega U_{dip} * \left(|\sum_{k=0}^m \alpha_k(t)\phi_k(x)|^2\right)\phi_i(x)\phi_j(x)dx$.
It's easy to see that A $B, C, D(\alpha)$ and $K(\alpha)$ are symmetric, and A $B, C, D(\alpha)$ can be directly calculated, while $K(\alpha)$ needs to estimate carefully
Let the convolution term $F(x,t) = U_{dip} * |\sum_{i=0}^m \alpha_i(t)\phi_i(x)|^2$. Notice

$$F(x,t) := \int_{x_0}^{x_m} \frac{|\sum_{i=0}^m \alpha_i(t)\phi_i(y)|^2}{|x-y|^\alpha}dy$$

$$= \alpha_0^2(t)\int_{x_0}^{x_1} \frac{\phi_0^2(y)}{|x-y|^\alpha}dy + \alpha_m^2(t)\int_{x_{m-1}}^{x_m} \frac{\phi_m^2(y)}{|x-y|^\alpha}dy$$

$$+ \sum_{i=1}^{m-1} \alpha_i^2(t)\int_{x_{i-1}}^{x_{i+1}} \frac{\phi_i^2(y)}{|x-y|^\alpha}dy + 2\sum_{0\le i<j\le m} \alpha_i(t)\alpha_j(t)\int_{x_0}^{x_m} \frac{\phi_i(y)\phi_j(y)}{|x-y|^\alpha}$$

FEM for the ground state of the 1D dipolar BEC

Setting that

$$L_i(x) := \int_{x_{i-1}}^{x_i} \frac{\phi_i^2(y)}{|x-y|^\alpha} dy = \frac{1}{h^2} \int_{x_{i-1}}^{x_i} \frac{(y-x+x-x_{i-1})^2}{|x-y|^\alpha} dy,$$

$$R_i(x) := \int_{x_i}^{x_{i+1}} \frac{\phi_i^2(y)}{|x-y|^\alpha} dy = \frac{1}{h^2} \int_{x_i}^{x_{i+1}} \frac{(x_{i+1}-x+x-y)^2}{|x-y|^\alpha} dy,$$

$$M_i(x) := \int_{x_i}^{x_{i+1}} \frac{\phi_i(y)\phi_{i+1}(y)}{|x-y|^\alpha} dy = \frac{1}{h^2} \int_{x_i}^{x_{i+1}} \frac{(x_{i+1}-y)(y-x_i)}{|x-y|^\alpha} dy.$$

then we have

$$F(x,t) = \alpha_0^2(t)R_0(x) + \sum_{i=1}^{m-1} \alpha_i^2(t)\big(L_i(x)+R_i(x)\big) + \alpha_m^2(t)L_m(x) +$$

$$2\sum_{i=0}^{m-1} \alpha_i(t)\alpha_{i+1}(t)M_i(x) \quad (7)$$

FEM for the ground state of the 1D dipolar BEC

Therefore $K(\alpha)_{ij} = \int_\Omega F(x,t)\phi_i(x)\phi_j(x)dx$ can be estimated. Then we have

$$A\vec{\alpha}'(t) = -\big(\frac{1}{2}B + C + \beta D(\vec{\alpha}) + \lambda K(\vec{\alpha})\big)\vec{\alpha}(t) \tag{8}$$

The initial condition $\psi(x,0) = \psi_0(x)$ shows that

$$\int_\Omega \psi_h(x,0)\phi_j(x)dx = \int_\Omega \psi_0(x)\phi_j(x)dx, \quad 0 \le j \le m, \tag{9}$$

and

$$A\vec{\alpha}(0) = \vec{b} \tag{10}$$

FEM for the ground state of the 1D dipolar BEC

Now we solve the ODEs (8) with the backward Euler scheme

$$\left[A+\tau\left(\frac{1}{2}B+C+\beta D(\vec{\alpha}^k)+\lambda K(\vec{\alpha}^k)\right)\right]\vec{\alpha}^{k+1}=A\vec{\alpha}^k \tag{11}$$

Furthermore,

$$\int_\Omega |\psi_h(x,t)|^2 dx=\vec{\alpha}^T A\vec{\alpha}\ ,0\le t\le t_0$$

After each discrete time level, $\psi_h(x,t)$ should be normalized to satisfy $\int_\Omega |\psi_h(x,t)|^2 dx=1$, that is,
$\psi_h(x,t):=\frac{\psi_h(x,t)}{\|\psi_h(x,t)\|}$.
In addition, the total energy can be rewritten

$$E(\psi_h(x,t))=\frac{1}{2}\vec{\alpha}^T B\vec{\alpha}+\vec{\alpha}^T C\vec{\alpha}+\frac{\beta}{2}\vec{\alpha}^T D(\vec{\alpha})\vec{\alpha}+\frac{\lambda}{2}\vec{\alpha}^T K(\vec{\alpha})\vec{\alpha} \tag{12}$$

FEM for the ground state of the 1D dipolar BEC

Proposition 1. Suppose the initial condition $\psi_0(x)$ is bounded uniformly and $\beta \geq 0$, then we have

$$\|\psi_h(x,t)\|_{L^2} \leq C, \tag{13}$$

where the constant C is independent of h and t.

Proposition 2. Suppose $\|\psi_{ht}(x,0)\|_{L^2}^2$ is bounded with respect to h uniformly and $\beta \geq \frac{4\lambda(2a)^{1-\alpha}}{1-\alpha}$, then we have

$$\|\psi_{ht}(x,t)\|_{L^2} \leq C, \tag{14}$$

where C is independent of h and t.

FEM for the ground state of the 1D dipolar BEC

Proposition 3. Under the assumptions of Proposition 1 and Proposition 2, we have

$$\begin{aligned} &\|\nabla\psi_h\|_{L^2} \le C, \quad \|V(x)|\psi_h|^2\|_{L^1} \le C, \\ &\|\psi_h\|_{L^4} \le C, \quad \|(U_{dip} * |\psi_h|^2)|\psi_h|^2\|_{L^1} \le C. \end{aligned} \tag{15}$$

Theorem 1. Under the assumptions of Proposition 1, 2, 3, there exists any $T > 0$ such that the finite element solution $\psi_h(x, t)$ is convergent to the generalized solution (4) on $[0, T]$.
The FEM for dynamical evolution of the 1D dipolar GPE is similar.

Summary

Example 1

The initial condition is chosen to be $\psi_0(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}$. The ground state $\psi_g := \psi_h^{k+1} = \sum_{j=0}^{m} \alpha_j^{k+1} \phi_j(x)$ is reached numerically when

$$\|\vec{\alpha}^{k+1} - \vec{\alpha}^{k}\|_\infty := \max_{0 \le j \le M} |\alpha_j^{k+1} - \alpha_j^{k}| \le \varepsilon := 10^{-6}.$$

We solve this problem on $[-16, 16]$ with $h = 1/8$ and $\tau = 0.01$.

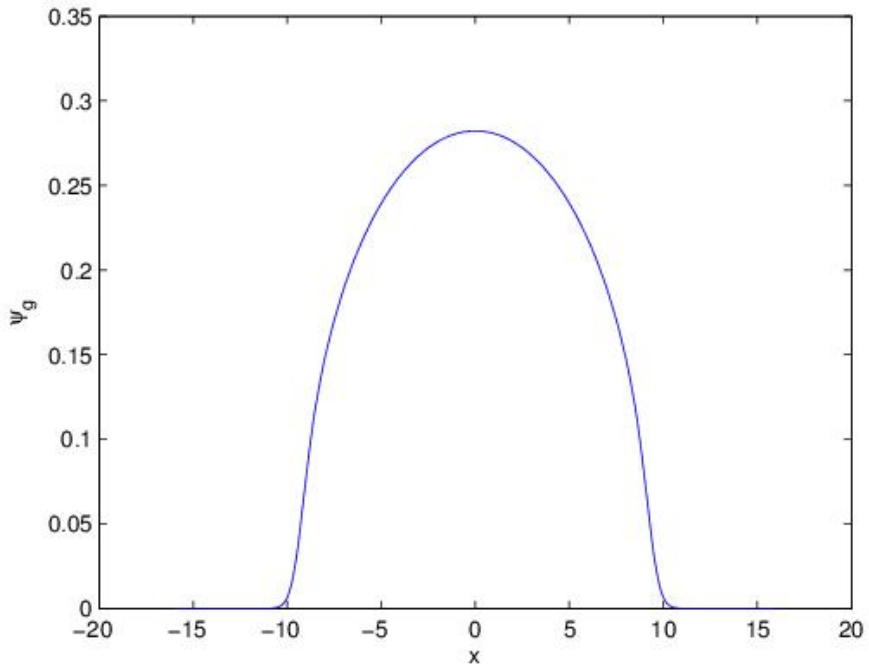


Fig.1. Ground state solution ψ_g .

Example 1

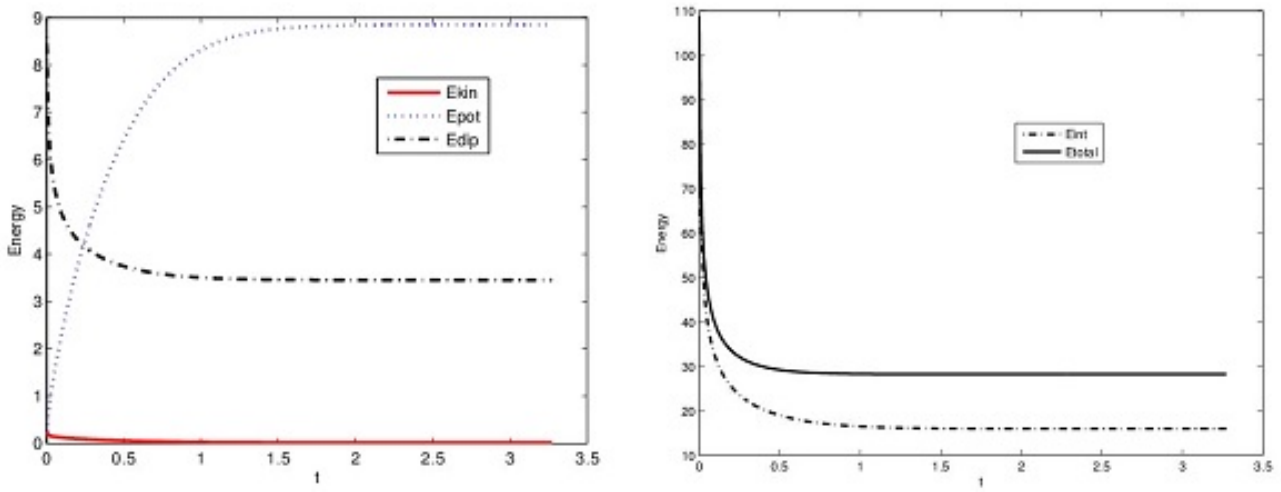


Fig.1. The energy evolution of a dipolar BEC with $\lambda = 10$ and $\beta = 500$.

Example 2

We solve this problem on $[-8, 8]$ with $h = 1/32$ and $\tau = 0.005$.

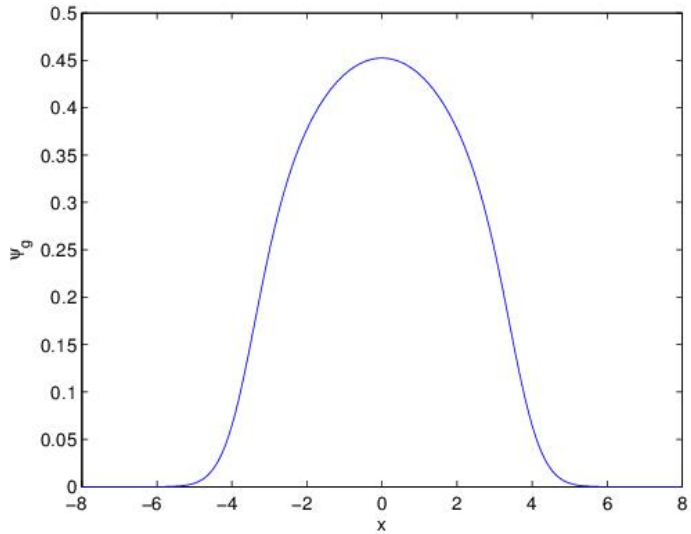
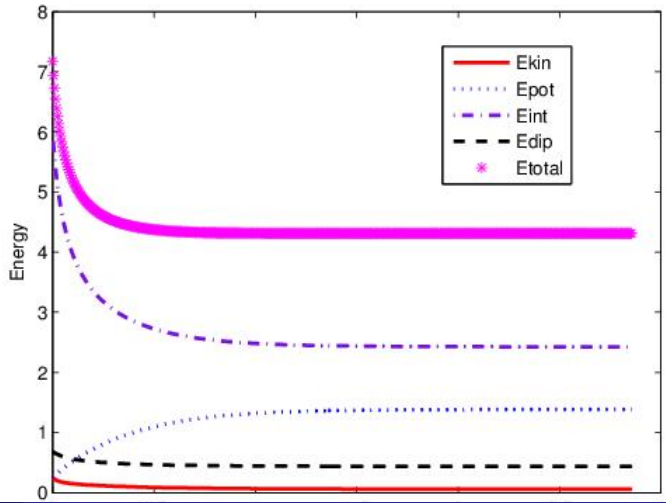


Fig.2. Ground state ψ_g and energy evolution with $\lambda = 0.8$ and $\beta = 30$.



Summary

Because the dipolar interaction is not only nonlinear but also nonlocal,the key difficulties are to efficiently and accurately calculate the nonlocal interaction and deal with singularity for numerical method. The convolution term can be split into a δ function (local) and directional derivative of potential (nonlocal), that is, the dipolar GPE is equivalent to the GPP:

$$
\begin{aligned}
i\psi_t(\mathbf{x},t) &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta-\lambda)|\psi|^2 - 3\lambda\partial_{\mathbf{ll}}(\omega(\mathbf{x},t))\right]\psi \quad (16)\\
\nabla^2\omega(\mathbf{x},t) &= -|\psi|^2, \quad (17)
\end{aligned}
$$

It also can be rewritten as follows:

$$
\begin{aligned}
i\psi_t(\mathbf{x},t) &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta-\lambda)|\psi|^2 + 3\lambda(\nabla(\mathbf{v}\cdot\mathbf{l})\cdot\mathbf{l})\right]\psi, \quad (18)\\
\nabla\cdot\mathbf{v} &= |\psi|^2, \mathbf{x}\in\mathbb{R}^3, t>0 \quad (19)\\
\mathbf{v} &= -\nabla\omega. \quad (20)
\end{aligned}
$$

Semi-discrete combined DG finite element method

total energy becomes

$$E(\psi(\mathbf{x},t)) =$$

$$\int_{\mathbb{R}^3}\left(\frac{1}{2}|\nabla\psi|^2+V(\mathbf{x})|\psi|^2+\frac{\beta-\lambda}{2}|\psi|^4\right)d\mathbf{x}+\frac{3\lambda}{2}\int_{\mathbb{R}^3}\nabla(\mathbf{v}\cdot\mathbf{l})\cdot\mathbf{l}|\psi|^2 d\mathbf{x}.$$

The whole space is usually truncated into a bounded computational domain Ω such as $\Omega=[-a,a]\times[-b,b]\times[-c,c]$ with homogeneous Dirichlet boundary condition for wave function ψ and the Neumann boundary condition for potential. In general, as $|\mathbf{x}|\longrightarrow\infty$, the wave function ψ tends to 0 fast, while the associated potential ω and its gradient $\mathbf{v}$ tend to 0 slowly. Then we replace equations (19) in $\mathbb{R}^3$ by the following equations in bounded domain Ω with the Neumann boundary condition

$$\nabla\cdot\mathbf{v}=|\psi|^2,\mathbf{v}\cdot\mathbf{n}|_{\partial\Omega}=\frac{1}{|\partial\Omega|}. \tag{21}$$

The boundary condition is chosen to avoid the inconsistency between the equation $\nabla\cdot\mathbf{v}=|\psi|^2$ and particle conservation.

$\int_\Omega\nabla\cdot\mathbf{v}d\mathbf{x}=\int_\Omega|\psi|^2 d\mathbf{x}=1$

Semi-discrete combined DG finite element method

Consider a regular partitioning of the domain Ω into polygonal elements K forming a mesh $\mathcal{T}_h$ satisfying the standard finite element conditions. Let $\varepsilon_h = \{e : e \text{ is an edge of } K \text{ for all } K \in \mathcal{T}_h\}$, $\varepsilon_h^0 = \{e : e \text{ is an interior edge of } K\}$ and $\varepsilon_h^\partial = \varepsilon_h \cap \partial\Omega$. We define that averages and jumps for scalar and vector function on $e \in \varepsilon^0$:

$$\overline{\psi} = \frac{1}{2}(\psi^{int} + \psi^{ext}), [\psi] = \psi^{int} - \psi^{ext}, \text{on } e \in \varepsilon^0,$$

where $\psi^{ext}(\psi^{int})$ represents ψ evaluated from outside (inside) of K.

Semi-discrete combined DG finite element method

Define finite element spaces:

$$C_h = \{\psi \in L^2(\Omega) : \psi|_K \in \mathbb{C}^k(K), \forall K \in \mathcal{T}_h\},$$

$$V_h = \{\mathbf{v} \in L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega) : \mathbf{v}|_K \in \mathbb{P}^k(K)\times\mathbb{P}^k(K)\times\mathbb{P}^k(K), \forall K \in \mathcal{T}_h\},$$

$$W_h = \{w \in L^2(\Omega) : w|_K \in \mathbb{P}^k(K), \forall K \in \mathcal{T}_h\}$$

and Lagrange multiplier ξ in the space

$$M_h = \{\eta \in L^2(\varepsilon_h) : \eta|_e \in \mathbb{P}^k(e), \forall e \in \varepsilon_h\}.$$

Then the DG finite element approximations ψ in C_h, $\mathbf{v}$ in V_h, ω in W_h, and ξ in M_h, are determined by requiring that

Semi-discrete combined DG finite element method

$$i\left\langle \psi_t, u\right\rangle_K = \frac{1}{2}\left\langle \nabla\psi, \nabla u\right\rangle_K - \frac{1}{2}\left\langle \widehat{\psi_n}, u\right\rangle_{\partial K} + \frac{1}{4}\left\langle [\psi], u_n\right\rangle_{\partial K} +$$

$$\left\langle V(\mathbf{x})\psi, u\right\rangle_K + (\beta-\lambda)\left\langle |\psi|^2\psi, u\right\rangle_K + \tag{22}$$

$$3\lambda\left\langle (\nabla(\mathbf{v}\cdot\mathbf{l})\cdot\mathbf{l})\psi(\mathbf{x},t), u\right\rangle_K,$$

$$\sum_{K\in\mathcal{T}_h}\left\langle \mathbf{v}, \mathbf{r}\right\rangle_K - \sum_{K\in\mathcal{T}_h}\left\langle \omega, \nabla\cdot\mathbf{r}\right\rangle_K + \sum_{K\in\mathcal{T}_h}\left\langle \xi, \mathbf{r}\cdot\mathbf{n}\right\rangle_{\partial K} = 0, \tag{23}$$

$$\sum_{K\in\mathcal{T}_h}\left\langle \nabla\cdot\mathbf{v}, p\right\rangle_K = \sum_{K\in\mathcal{T}_h}\left\langle |\psi|^2, p\right\rangle_K, \tag{24}$$

$$\sum_{K\in\mathcal{T}_h}\left\langle \mathbf{v}\cdot\mathbf{n}, \eta\right\rangle_{\partial K} = \left\langle \frac{1}{|\partial\Omega|}, \eta\right\rangle_{\partial\Omega}. \tag{25}$$

property of Semi-discrete combined DG

The numerical fluxes for ψ by direct DG method are chosen as:

$$\widehat{\psi_n} = \alpha_0 \frac{[\psi]}{|e|} + \overline{\nabla\psi \cdot \mathbf{n}} \tag{26}$$

We have

Theorem 2. The scheme (23)-(25) keeps the particle conservation,

$$\|\psi(\mathbf{x},t)\|^2 = \int_{\mathbb{R}^3} |\psi(\mathbf{x},t)|^2 \, d\mathbf{x} = \|\psi(\mathbf{x},0)\|^2 = 1.$$

Combined DG method for ground state

In order to obtain the ground states, we take the ansatz

$$\psi(\mathbf{x}, t) = e^{-i\mu t}\phi(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \quad t \geq 0, \mu \in \mathbb{R} \tag{27}$$

Inserting (27) into the system (18)-(20), we get the time-independent GP equation or the eigenvalue problem

$$\begin{aligned} \mu\phi(\mathbf{x}) &= [-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta - \lambda)|\phi(\mathbf{x})|^2 + 3\lambda(\nabla(\mathbf{v}\cdot\mathbf{I})\cdot\mathbf{I})]\phi(\mathbf{x}), \\ \mathbf{v} &= -\nabla\omega, \nabla\cdot\mathbf{v} = |\phi|^2, \mathbf{x} \in \mathbb{R}^3 \end{aligned} \tag{28}$$

under the constraint

$$\|\phi\| = \sqrt{\int_{\mathbf{x}\in\mathbb{R}^3} |\phi(\mathbf{x})|^2 d\mathbf{x}} = 1. \tag{29}$$

Combined DG method for ground state

Find $\phi_g \in S$ and $\mu_g \in \mathbb{R}$ such that

$$E^g := E(\phi_g) = \min_{\phi \in S} E(\phi), \qquad \mu^g := \mu(\phi_g), \tag{30}$$

S is defined as

$$S := \{\phi(\mathbf{x}) \mid \ \|\phi\| = 1, \ E(\phi) < \infty\}. \tag{31}$$

and eigenvalue of (28)is defined as

$$\begin{aligned}
\mu(\phi) &= \int_{\mathbb{R}^3} [\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + (\beta - \lambda)|\phi|^4 + 3\lambda(\nabla(\mathbf{v}\cdot\mathbf{l})\cdot\mathbf{l})|\phi|^2] d\mathbf{x} \\
&\equiv E(\phi) + \int_{\mathbb{R}^3} \frac{1}{2}[(\beta - \lambda)|\phi|^4 - 3\lambda(\nabla(\mathbf{v}\cdot\mathbf{l})\cdot\mathbf{l})|\phi|^2] d\mathbf{x}, \\
\mathbf{v} &= -\nabla\omega, \nabla\cdot\mathbf{v} = |\phi|^2 .
\end{aligned}$$

Combined DG method for ground state

The function $\phi(\mathbf{x}, t)$ is the solution of the following gradient flow with discrete normalization:

$$-\frac{\partial \phi}{\partial t} = [-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta - \lambda)|\phi|^2 + 3\lambda(\nabla(\mathbf{v}\cdot\mathbf{I})\cdot\mathbf{I})]\phi, \quad (32)$$

$$\mathbf{v} = -\nabla\omega, \nabla\cdot\mathbf{v} = |\phi|^2, \mathbf{x}\in\Omega, t\in(t_n, t_{n+1}), \quad (33)$$

$$\phi(\mathbf{x}, t)|_{\partial\Omega} = 0,\ \mathbf{v}\cdot\mathbf{n}|_{\partial\Omega} = \frac{1}{|\partial\Omega|}, t\geq 0, \quad (34)$$

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}),\ \|\phi_0\| = 1, \quad (35)$$

$$\phi(\mathbf{x}, t_{n+1}) := \phi(\mathbf{x}, t_{n+1}^+) = \frac{\phi(\mathbf{x}, t_{n+1}^-)}{\|\phi(\cdot, t_{n+1}^-)\|},\ \mathbf{x}\in\Omega,\ n\geq 1, \quad (36)$$

DG for ground state

From time t_n to t_{n+1}, the combined DG with Euler backward discretization in time for (32)-(33) is to find ϕ in C_h, $\mathbf{v}$ in V_h, ω in W_h, and ξ in M_h such that the following

$$
\begin{aligned}
-\langle \phi_t, u\rangle_K &= \frac{1}{2}\langle \nabla\phi, \nabla u\rangle_K - \frac{1}{2}\left\langle \widehat{\phi_n}, u\right\rangle_{\partial K} + \frac{1}{4}\langle [\phi], u_n\rangle_{\partial K} + \\
&\quad \langle V(\mathbf{x})\phi, u\rangle_K + (\beta-\lambda)\left\langle |\phi^n|^2\phi, u\right\rangle_K \\
&\quad +3\lambda\langle (\nabla(\mathbf{v}\cdot\mathbf{l})\cdot\mathbf{l})\psi(\mathbf{x},t), u\rangle_K ,\\
\sum_{K\in\mathcal{T}_h}\langle \mathbf{v}, \mathbf{r}\rangle_K &= \sum_{K\in\mathcal{T}_h}\langle \omega, \nabla\cdot\mathbf{r}\rangle_K - \sum_{K\in\mathcal{T}_h}\langle \xi, \mathbf{r}\cdot\mathbf{n}\rangle_{\partial K} ,\\
\sum_{K\in\mathcal{T}_h}\langle \mathbf{v}, \nabla p\rangle_K &= \sum_{K\in\mathcal{T}_h}\left\langle |\phi^n|^2, p\right\rangle_K ,\\
\sum_{K\in\mathcal{T}_h,}\langle \mathbf{v}\cdot\mathbf{n}, \eta\rangle_{\partial K} &= \left\langle \frac{1}{|\partial\Omega|}, \eta\right\rangle_{\partial\Omega} ,
\end{aligned}
$$

hold for any u in C_h, $\mathbf{r}$ in V_h, p in W_h, and η in M_h .

A semi-implicit time discretization for dynamic evolution

Turn to deal with the semi-discrete system for dynamic evolution. This finite element scheme (23)-(25)is nonlinear ODEs. First solve velocity field (24)-(25) to get v,then integrate the nonlinear ODEs exactly in time. The scheme (24)-(25) can be written into a matrix equation

$$\begin{pmatrix} A & -B & C \\ B^t & 0 & 0 \\ C^t & 0 & 0 \end{pmatrix} \begin{pmatrix} Q \\ W \\ \Xi \end{pmatrix} = \begin{pmatrix} 0 \\ F \\ G_n \end{pmatrix}, \tag{37}$$

Both the vectors of Q and W can now be easily eliminated to obtain an equation for the multiplier only, namely,

$$\mathbb{D}\Xi = \mathbb{H}, \tag{38}$$

where $\mathbb{D}$ and $\mathbb{H}$ are given by

$$\mathbb{D} = C^t(SM^{-1}S^t - A^{-1})C,$$
$$\mathbb{H} = G_n - C^t SM^{-1}F,$$
$$M = B^t A^{-1}B,\ S = A^{-1}B.$$

A semi-implicit time discretization for dynamic evolution

We substitute the gradient $\mathbf{v}$ in equation (23) and sum it over all elements to get

$$i \sum_{K \in \mathcal{T}_h} \langle \psi_t, u \rangle_K =$$

$\sum_{K \in \mathcal{T}_h} \frac{1}{2} \langle \nabla \psi, \nabla u \rangle_K +$
$\sum_{e \in \varepsilon_h^{\partial},} \left(\frac{1}{2} \langle [\psi], [u] \rangle_e + \frac{1}{2} \left\langle \overline{\nabla \psi \cdot \mathbf{n}} [u] \right\rangle_e + \frac{1}{2} \left\langle [\psi] \overline{\nabla u \cdot \mathbf{n}} \right\rangle_e \right)$
$+ \sum_{K \in \mathcal{T}_h} \left(\langle V(\mathbf{x}) \psi, u \rangle_K + (\beta - \lambda) \left\langle |\psi^n|^2 \psi, u \right\rangle_K + 3\lambda \langle (\nabla(\mathbf{v} \cdot \mathbf{l}) \cdot \mathbf{l}) \psi, u \rangle_K \right).$

Write it into the global linear ODE system by inverting the mass matrix:

$$\frac{d\mathbf{\Psi}}{dt} = \mathbf{G}\mathbf{\Psi}, \tag{39}$$

We integrate the equation (40) exactly from time t^n to t^{n+1} and get

$$\mathbf{\Psi}^{n+1} = e^{\mathbf{G}\Delta t} \mathbf{\Psi}^n, \tag{40}$$

The Krylov subspace approximation is adopted

$$e^{G\Delta t} \mathbf{\Psi}^n = \beta \mathbf{V}_{m+1} e^{\triangle t \overline{\mathbf{H}}_{m+1}} \mathbf{e}_1 \tag{41}$$

A semi-implicit time discretization for dynamic evolution

The orthonormal basis and the upper Hessenberg matrix resulting from the following Arnoldi process:

Algorithm 1

$\overline{\mathbf{H}}_{m+2} = zeros[m+2, m+2]$;

1. Compute the initial vector: $\mathbf{v}_1 = \mathbf{\Psi}^n / \|\mathbf{\Psi}^n\|_2$;
2. Perform iterations: Do $j = 1, 2, \ldots, m$:
   (1) Compute the vector $\mathbf{p} = G\mathbf{v}_j$;
   (2) Do $i = 1, 2, \ldots, j$:
      (2.1) Compute the inner product $h_{ij} = (\mathbf{p}, \mathbf{v}_i)$;
      (2.2) Compute the vector $\mathbf{p} = \mathbf{p} - h_{ij}\mathbf{v}_i$;
   (3) Compute $h_{j+1,j} = \|\mathbf{p}\|_2$;
   (4) If $h_{j+1,j} = 0$, then stop the iteration;
      Else compute the next basis vector $\mathbf{v}_{j+1} = \mathbf{p}/h_{j+1,j}$.
3. $\overline{\mathbf{H}}(m+2, m+1) = 1$.

Summary

Numerical results for the 3D problem

Here we apply the combined DG method to compute the ground states and dynamics of dipolar BEC in the three-dimensional (3D) space with hexahedra mesh.The combined DG method is applied with the lowest-order Raviart-Thomas element for the solution of Poisson equation. In solving the linear algebra equations, we use the Conjugate Gradient (CG) method. The ground states reached numerically when

$$\|\psi^{(k+1)} - \psi^{(k)}\|_\infty := \max_{K\in\mathcal{T}_h} |\psi^{(k+1)} - \psi^{(k)}| \le \varepsilon = 10^{-6}.$$

The DDG method for the computing of GP equation is applied with linear element. The time step is chosen as $\Delta t = 10^{-3}$ in the computation.

Example 3.Ground states of dipolar BECs

We take the bounded computation domain $\Omega = [-8, 8]^3$ with the Neumann boundary condition. The dipolar direction is fixed with $\mathbf{l} = (0, 0, 1)^T$,the harmonic potential $V(\mathbf{x}) = \frac{1}{2}\left(x^2 + y^2 + 0.25z^2\right)$ and $\beta = 207.16$, $\lambda = 33.146$. The 'exact' values for the energy and chemical are $E^g = 2.72842$ and $\mu^g = 3.58331$ which is found using P^2 element and a $64 \times 64 \times 64$ mesh. We adopt it as the reference value and chose the relative error in the energy as the measure of the discretization error.

Table 1
Spatial errors of energy and chemical potential for the ground state of dipolar BEC for $\beta = 207.16$ and $\lambda = 33.146$.

Mesh	$8 \times 8 \times 8$	$16 \times 16 \times 16$	$32 \times 32 \times 32$	$64 \times 64 \times 64$
err_E	3.51e−3	1.01e−3	2.51e−4	5.91e−5
err_μ	5.17e−3	1.32e−3	3.72e−4	9.18e−5

Example 3. Ground states of dipolar BECs with different potentials

Consider the following three different potentials, i.e. that harmonic potential

$$V(\mathbf{x}) = \frac{1}{2}\left(x^2 + y^2 + z^2\right),$$

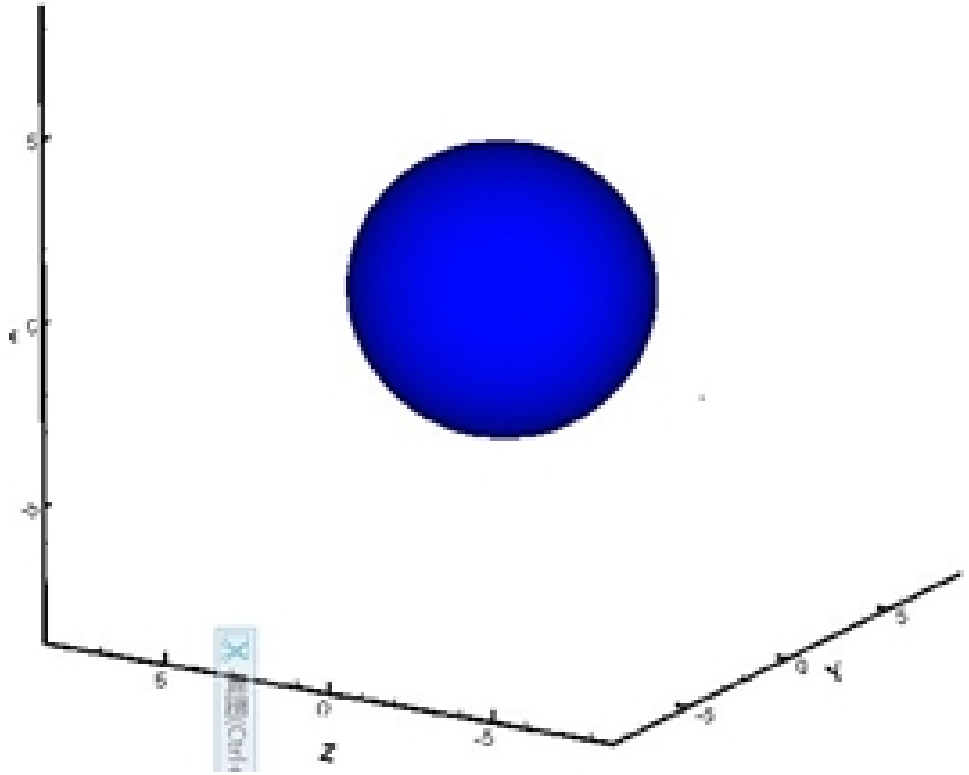
double-well potential

$$V(\mathbf{x}) = \frac{1}{2}\left(x^2 + y^2 + z^2\right) + 4e^{-z^2/2},$$

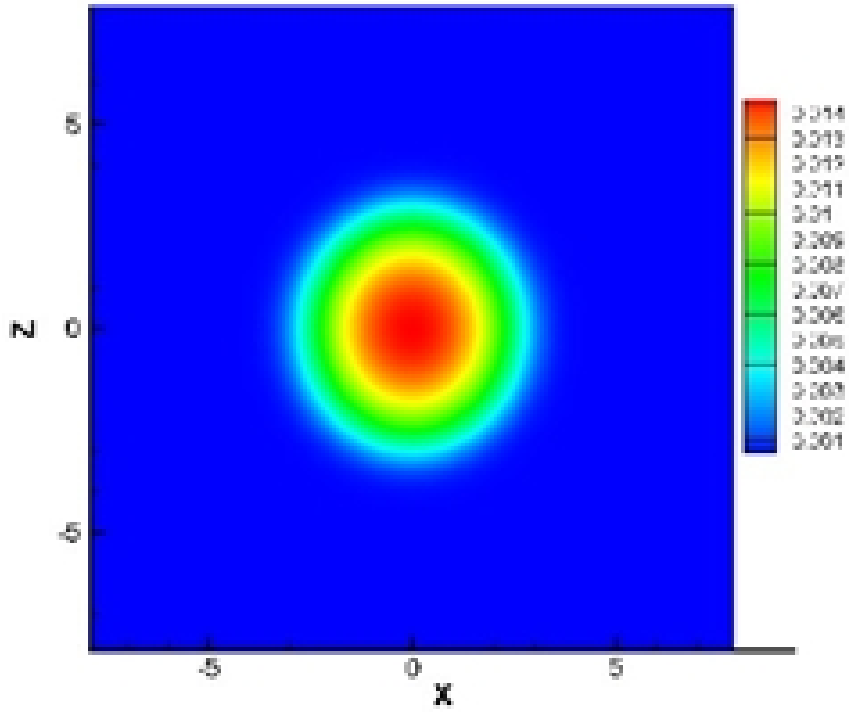
and optical lattice potential,

$$V(\mathbf{x}) = \frac{1}{2}(x^2 + y^2 + z^2) + 100\left(\sin^2(\frac{\pi x}{2}) + \sin^2(\frac{\pi y}{2}) + \sin^2(\frac{\pi z}{2})\right).$$

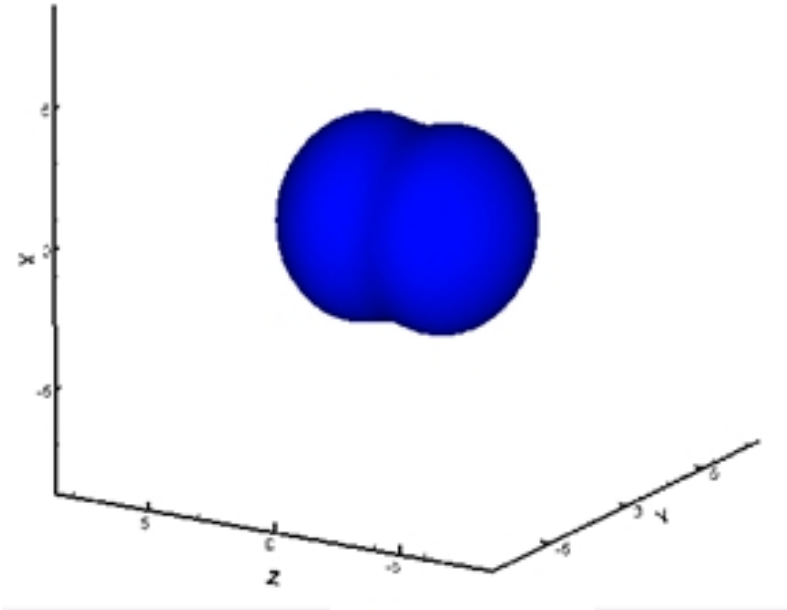
The initial condition is $\phi_0(x, y, z) = \pi^{-3/4} e^{-\left(x^2+y^2+z^2\right)}$. **Figure 3** depicts the ground state ϕ_g, i.e., the isosurface of $|\phi_g| = 0.01$ and slice view of $\phi_g(x, 0, z)$.



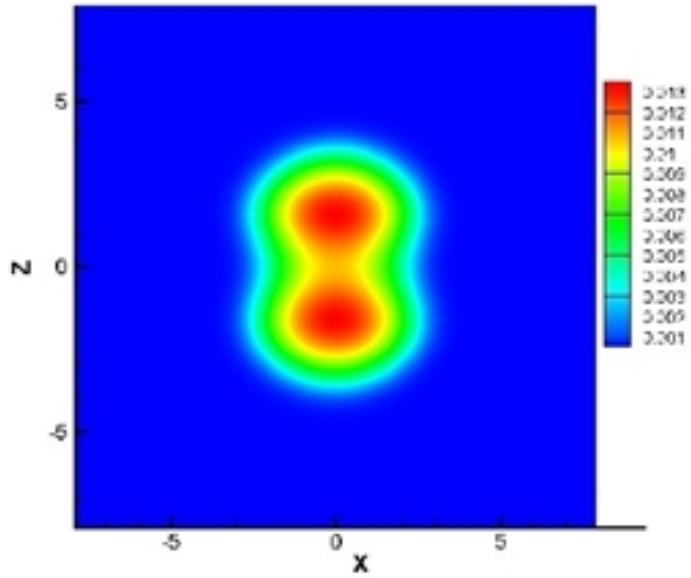
(a)



(b)



(c)



(d)

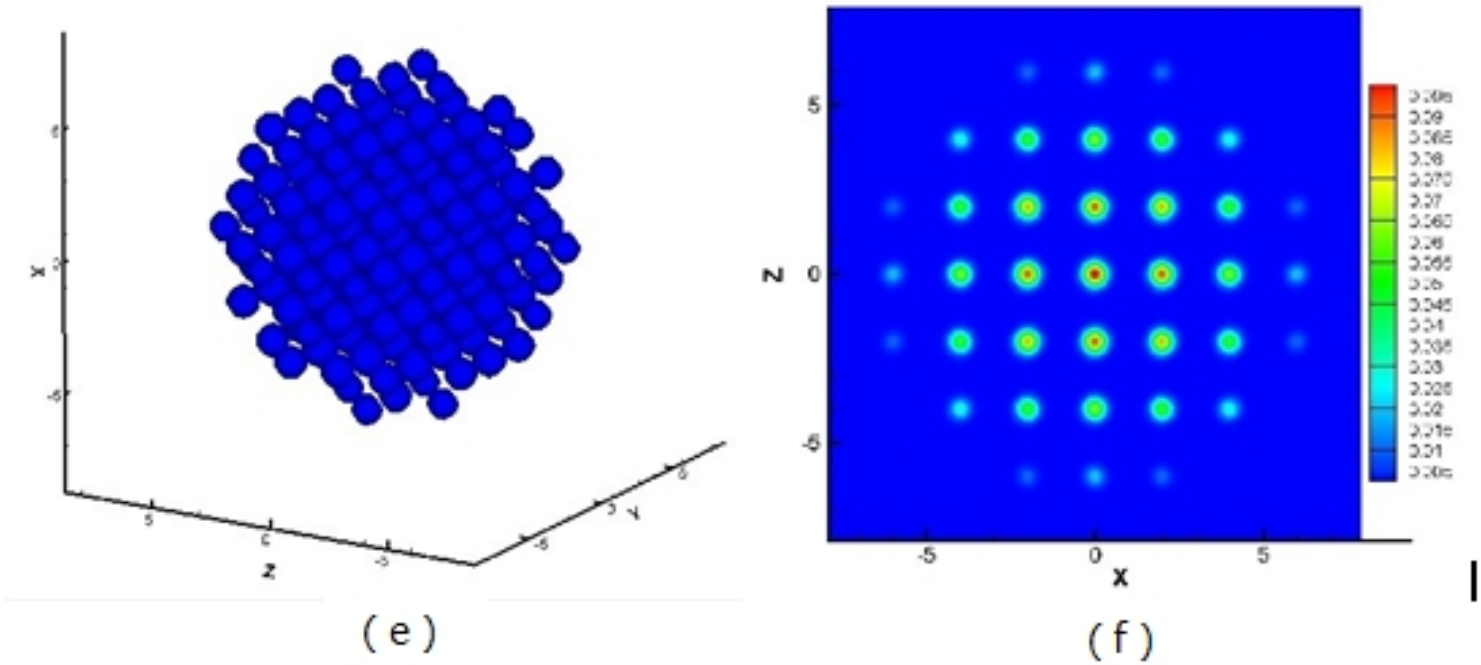


Fig.3. Surface plots of ground state $|\phi_g(x,0,z)|^2$ (right column) and isosurface plots of $|\phi_g(x,0,z)| = 0.01$ (left column) of a dipolar BEC under harmonic potential (top row), double-well potential (middle row) and optical lattice potential (bottom row).

Example 4.Dynamics of dipolar BECs

Now we study the dynamics behaviors 3D dipolar BEC system with dipolar direction $\mathbf{l} = (0, 0, 1)^T$, potential $V(\mathbf{x}) = \frac{1}{2}\left(x^2 + y^2 + 25z^2\right)$, $\beta = 103.58$ and $\lambda = 82.864$. We take the bounded computational domain $[-8, 8]^2 \times [-4, 4]$. **Table 2** shows the L^2 and maximum norm errors, e.g. $\|e\|_{L^2}$ and $\|e\|_\infty$, with different meshes at t=0.8.

Table 2
Spatial errors of ψ for Case 1 at $t = 0.8$.

$N_x \times N_y \times N_z$	$8 \times 8 \times 4$	$16 \times 16 \times 8$	$32 \times 32 \times 16$	$64 \times 64 \times 32$
$\|e\|_{L^2}$	1.10e−1	2.57e−2	6.48e−3	1.60e−3
$\|e\|_\infty$	2.43e−2	6.01e−3	1.51e−3	3.75e−4

From **Fig. 4(a)**, we can see that semi-implicit time discretization demonstrate the one-order convergence rate in time.The DG method can approximate the particle very well(up to 6 significant digits,cf **Figure 4(b)**).

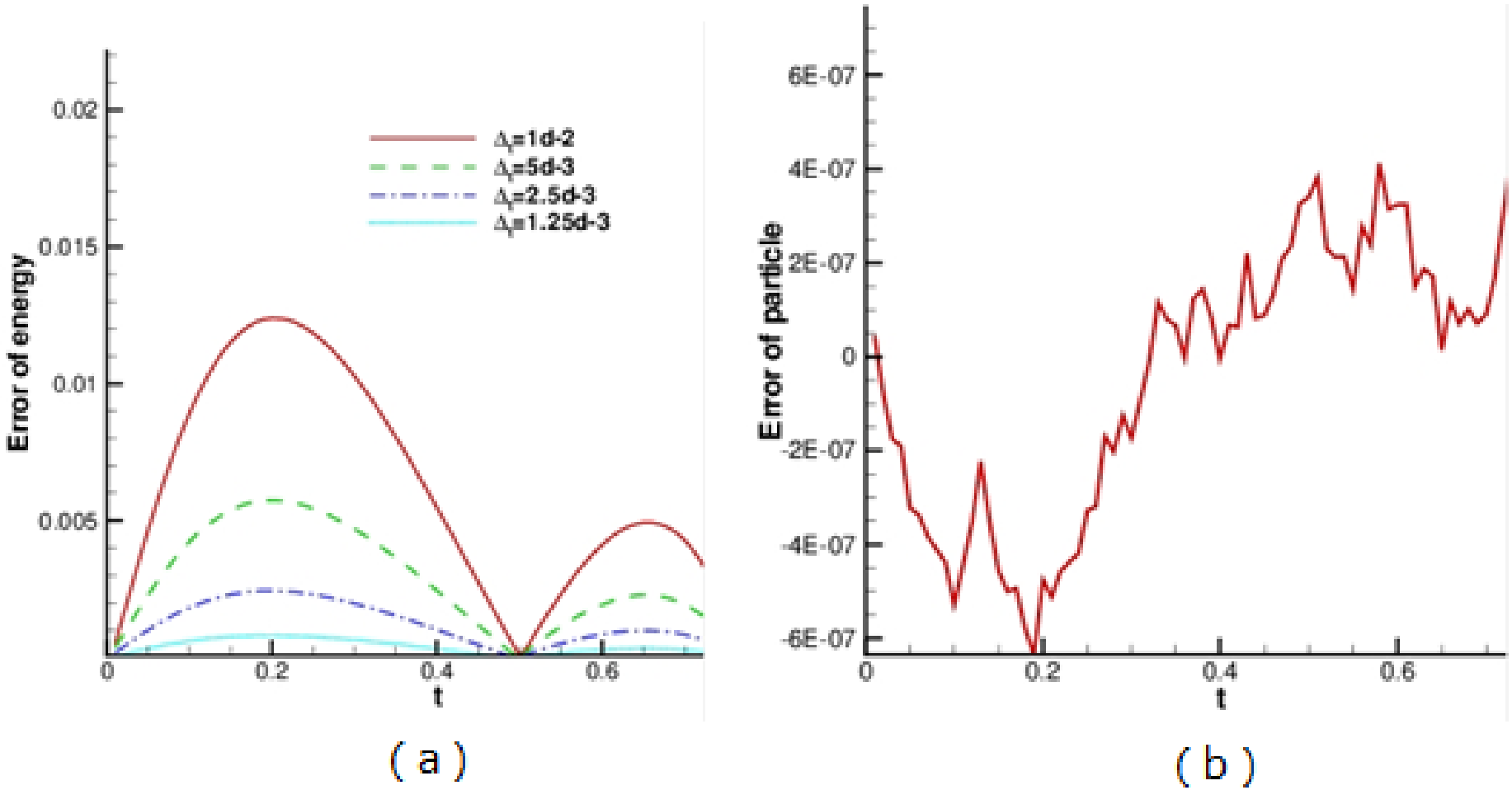


Fig.4. Time evolution of the errors between the discretized energy and particle

Case 1

Study the dynamics of suddenly changing the dipolar direction from $\mathbf{l} = (0, 0, 1)^T$ to $\mathbf{l} = (1, 0, 0)^T$ at $t = 0$. The time evolution of kinetic energy $E_{kin}(\psi)$, potential energy $E_{pot}(\psi)$, interaction energy $E_{int}(\psi)$, dipolar energy $E_{dip}(\psi)$ and total energy $E(\psi)$ are plotted in **Fig. 5 (a)**. We can also observe that the total energy conserved very well. The isosurface of density function $|\psi(\mathbf{x}, t)|^2 = 0.01$ are plotted in **Fig. 6** at time $t = 0,\ 1,\ 2,\ 3$. The results agree well with the reference spectral results in.

Case 2

study the dynamics of a dipolar BECs when the trap potential is suddenly changed from $\frac{1}{2}(x^2 + y^2 + 25z^2)$ to $\frac{1}{2}(x^2 + y^2 + z^2)$ at time $t = 0$. **Fig. 5 (b)** plots time evolution of kinetic energy $E_{kin}(\psi)$, potential energy $E_{pot}(\psi)$, interaction energy $E_{int}(\psi)$, dipolar energy $E_{dip}(\psi)$ and total energy $E(\psi)$. From **Fig. 5 (a) and (b)**, one can see that the total energy keeps conservation well for **Case 1 and 2**. The isosurface plots of density $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at time $t = 0,\ 1,\ 2,\ 3$. for dipolar BECs are plotted in **Fig. 7**.

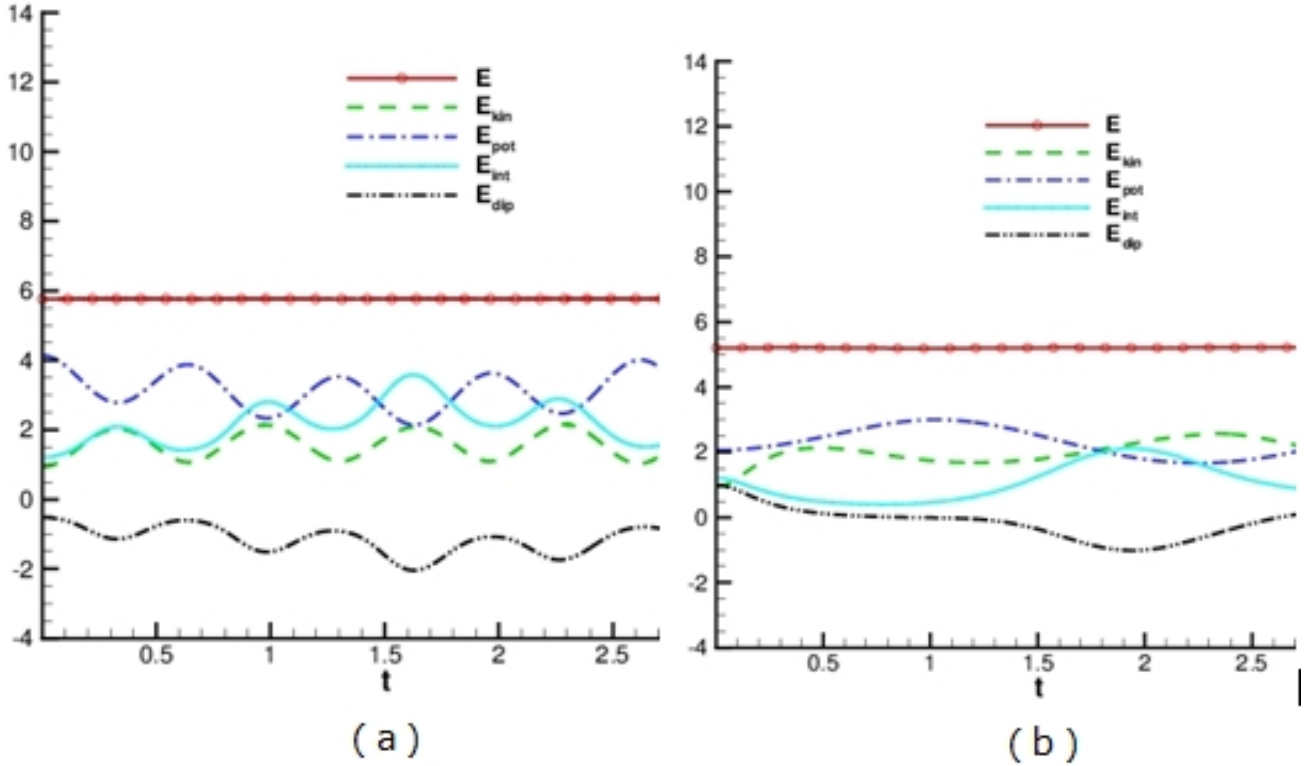
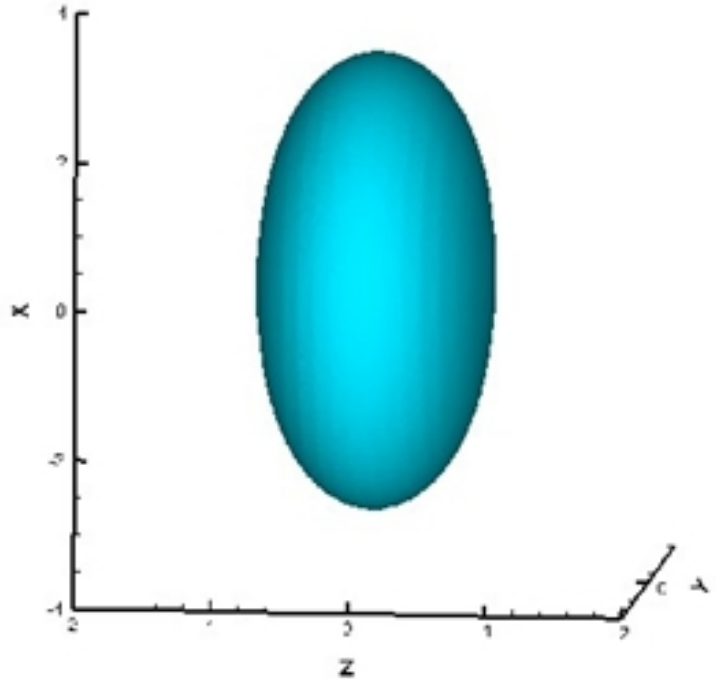
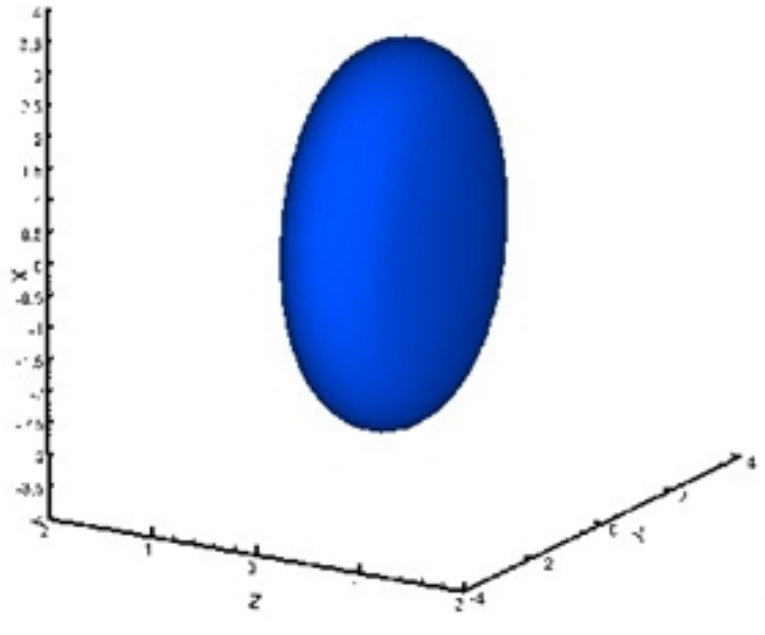


Fig.5. Time evolution of different energy quantities for (a) **Case 1**, (b) **Case 2** of dynamics of dipolar BECs.



(a)



(b)

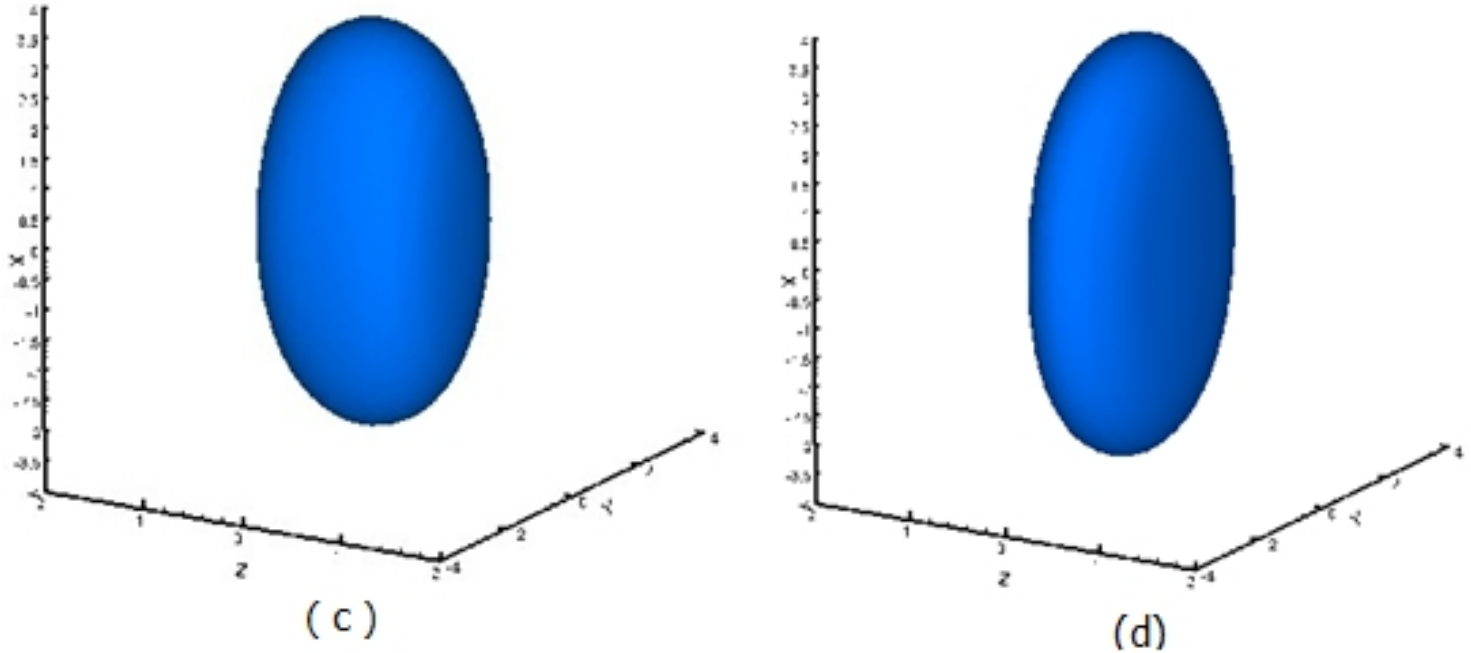
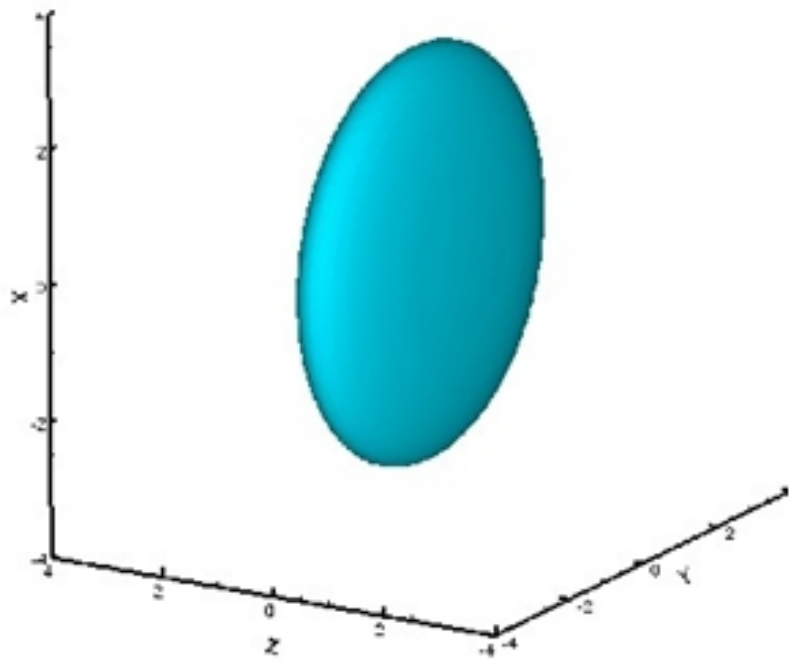
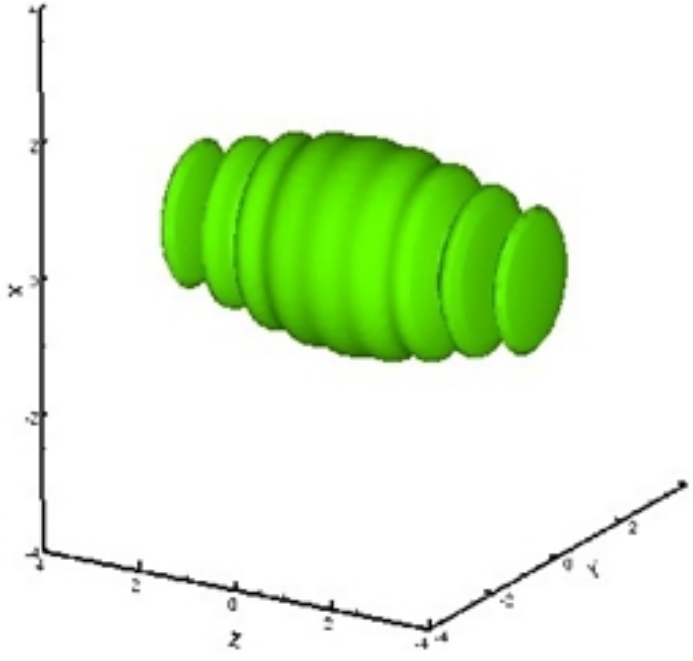


Fig.6. The isosurface plots of density $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at (a) $t = 0$, (b) $t = 1$, (c) $t = 2$, (d) $t = 3$ for dipolar BECs with the dipolar direction changing from $\mathbf{n} = (0, 0, 1)^T$ to $(1, 0, 0)^T$ suddenly at time $t = 0$.



(a)



(b)

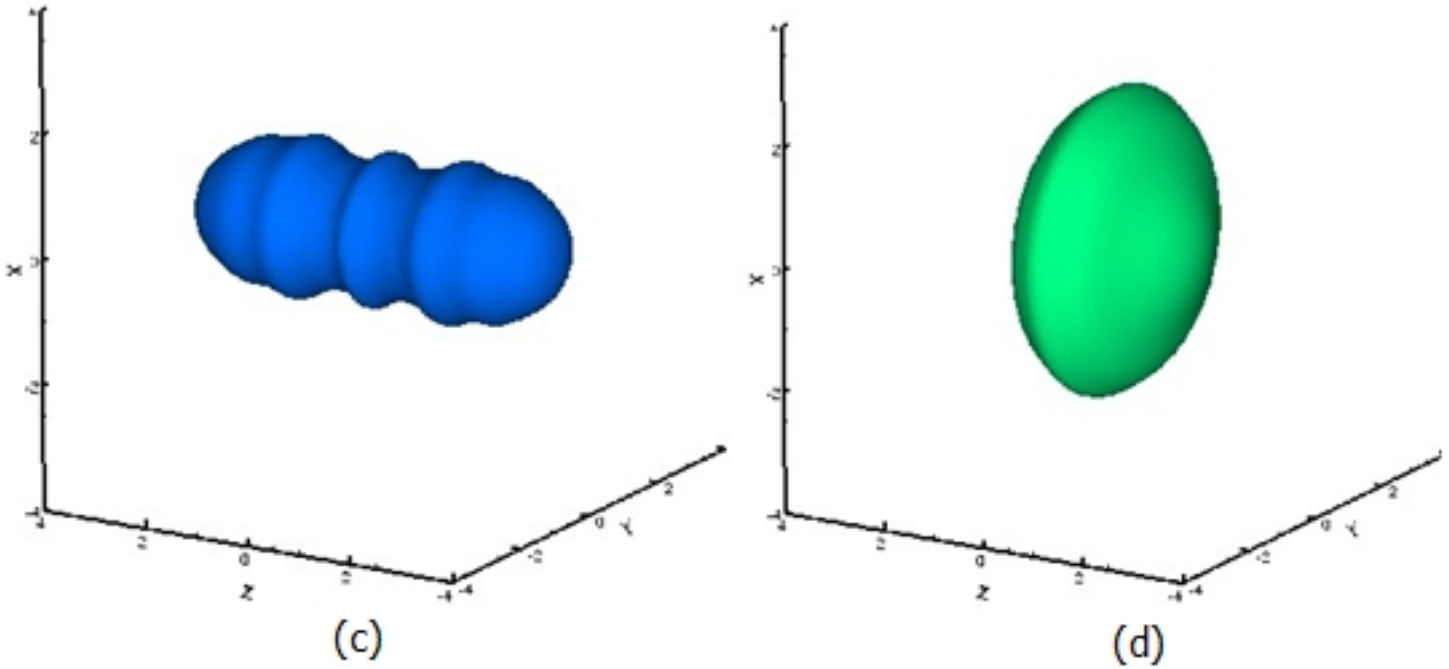


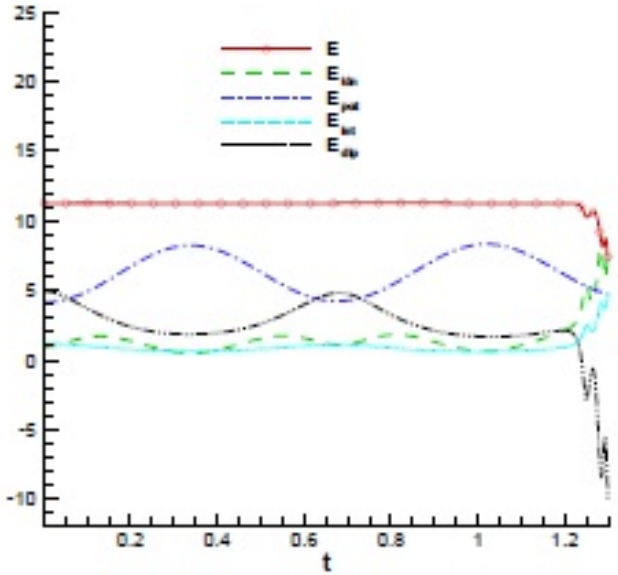
Fig.7. The isosurface plots of density $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at (a) $t = 0$, (b) $t = 1$, (c) $t = 2$, (d) $t = 3$ for dipolar BECs with the trap potential $V(\mathbf{x})$ changing from $\frac{1}{2}(x^2 + y^2 + 25z^2)$ to $\frac{1}{2}(x^2 + y^2 + z^2)$ suddenly at time $t = 0$.

Case 3

study the collapse of dipolar BEC with changing the dipolar interaction from $\lambda = 82.864$ to $\lambda = 414.32$ suddenly at $t = 0$. **Fig. 8 (c)** plots time evolution of kinetic energy $E_{kin}(\psi)$, potential energy $E_{pot}(\psi)$, interaction energy $E_{int}(\psi)$, dipolar energy $E_{dip}(\psi)$ and total energy $E(\psi)$. The isosurface of density function $|\psi(\mathbf{x}, t)|^2 = 0.01$ are plotted in **Fig. 9** at time $t = 0,\ 0.7,\ 1.1,\ 1.3$.

Case 4

study the collapse of dipolar BEC with changing the interaction constant β from $\beta = 103.58$ to $\beta = -569.69$ suddenly at $t = 0$. **Fig. 8 (d)** plots time evolution of kinetic energy $E_{kin}(\psi)$, potential energy $E_{pot}(\psi)$, interaction energy $E_{int}(\psi)$, dipolar energy $E_{dip}(\psi)$ and total energy $E(\psi)$. The isosurface of density function $|\psi(\mathbf{x}, t)|^2 = 0.01$ are plotted in **Fig. 10** at time $t = 0,\ 0.1,\ 0.15,\ 0.20$.



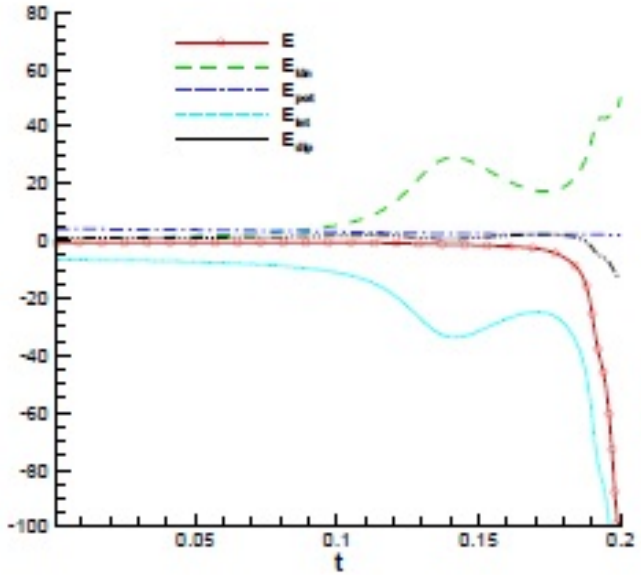
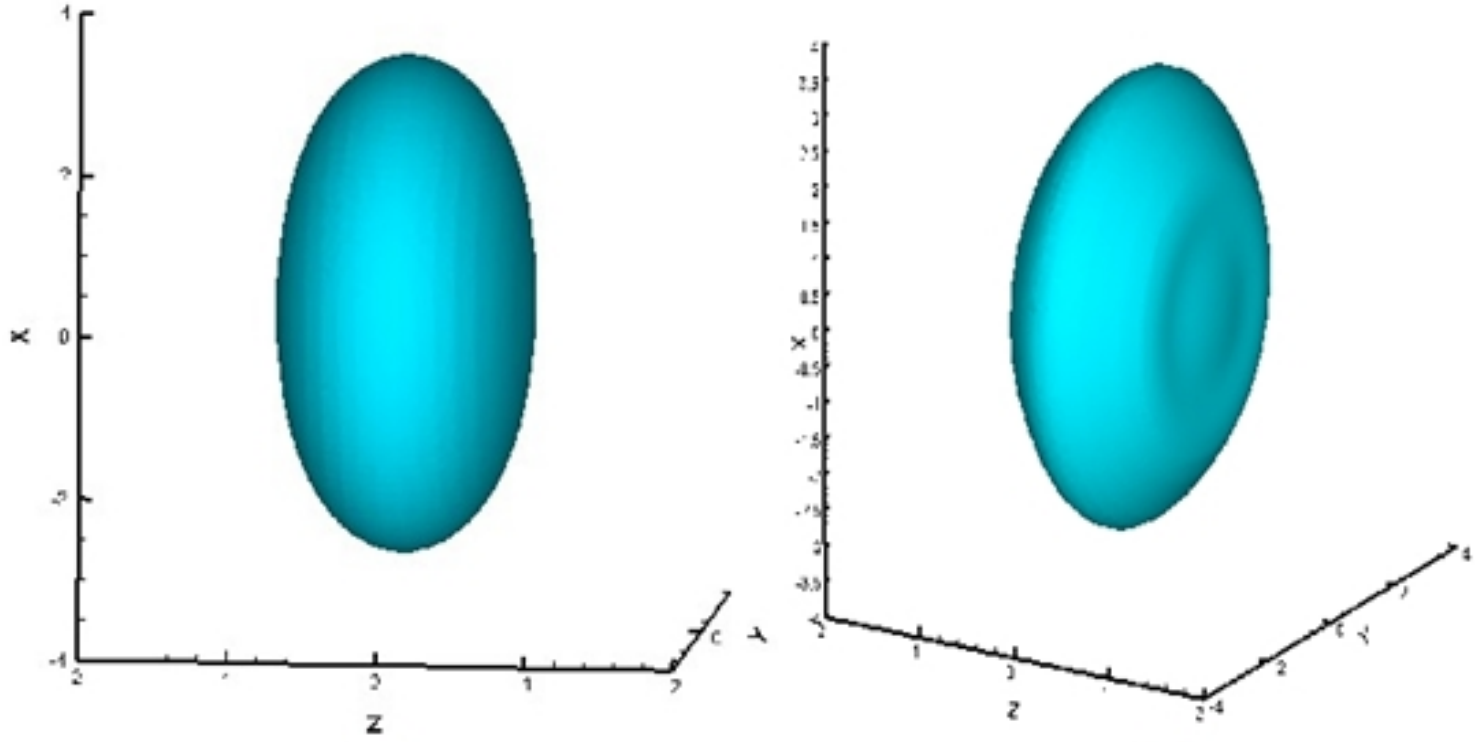


Fig.8. Time evolution of different energy quantities for (c) **Case 3** and (d) **Case 4** of dynamics of dipolar BECs.



(a) (b)

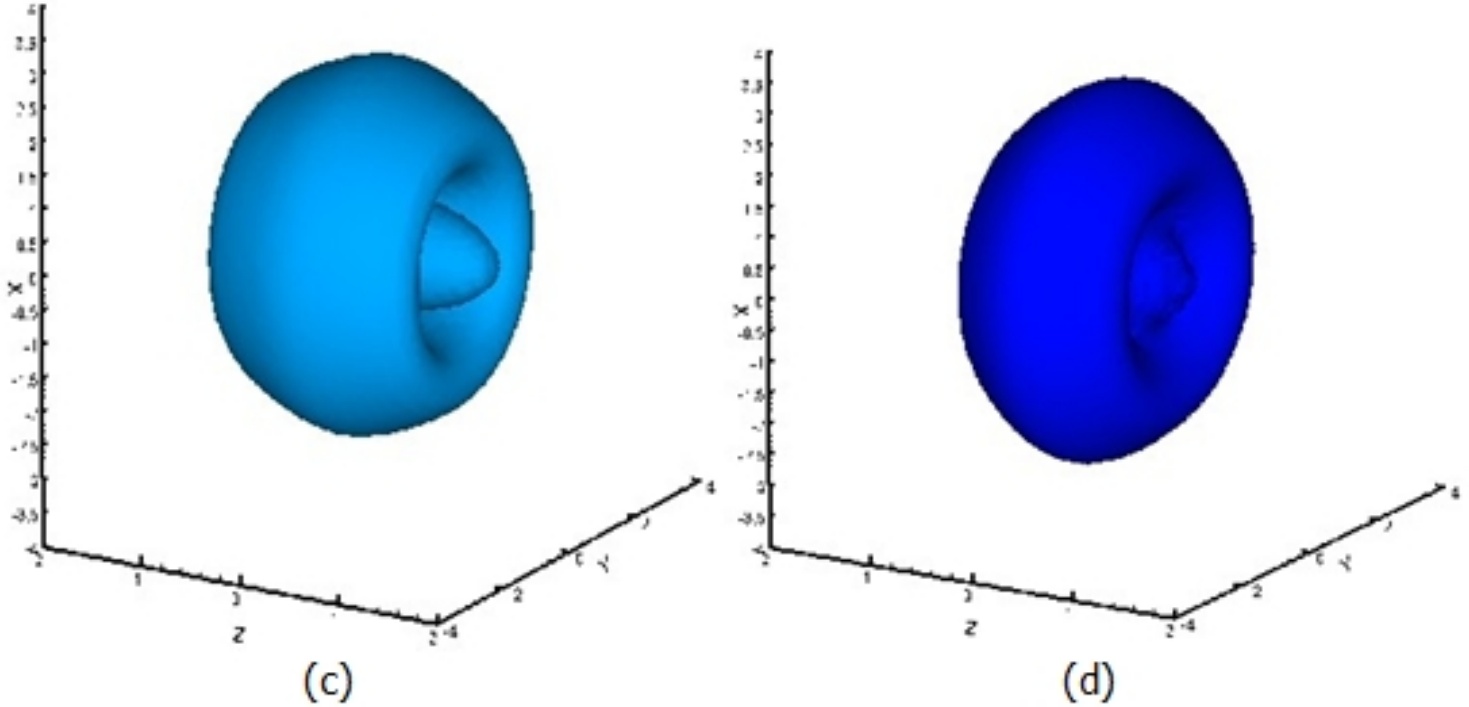
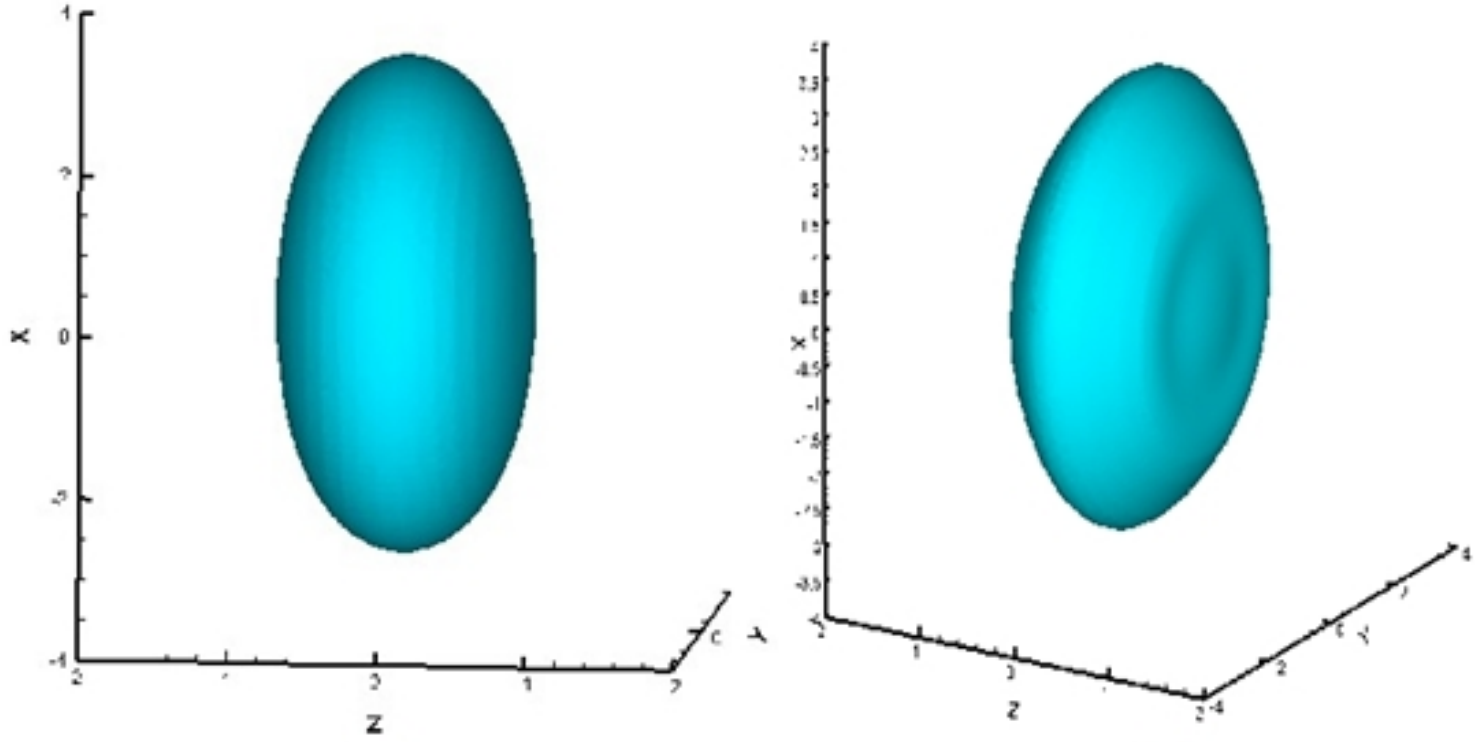


Fig.9. The isosurface plots of density $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at (a) $t = 0.0$, (b) $t = 0.7$, (c) $t = 1.1$, (d) $t = 1.3$ for dipolar BECs with the dipolar interaction constant λ changing from 82.864 to 414.32 suddenly at time $t = 0$.



(a) (b)

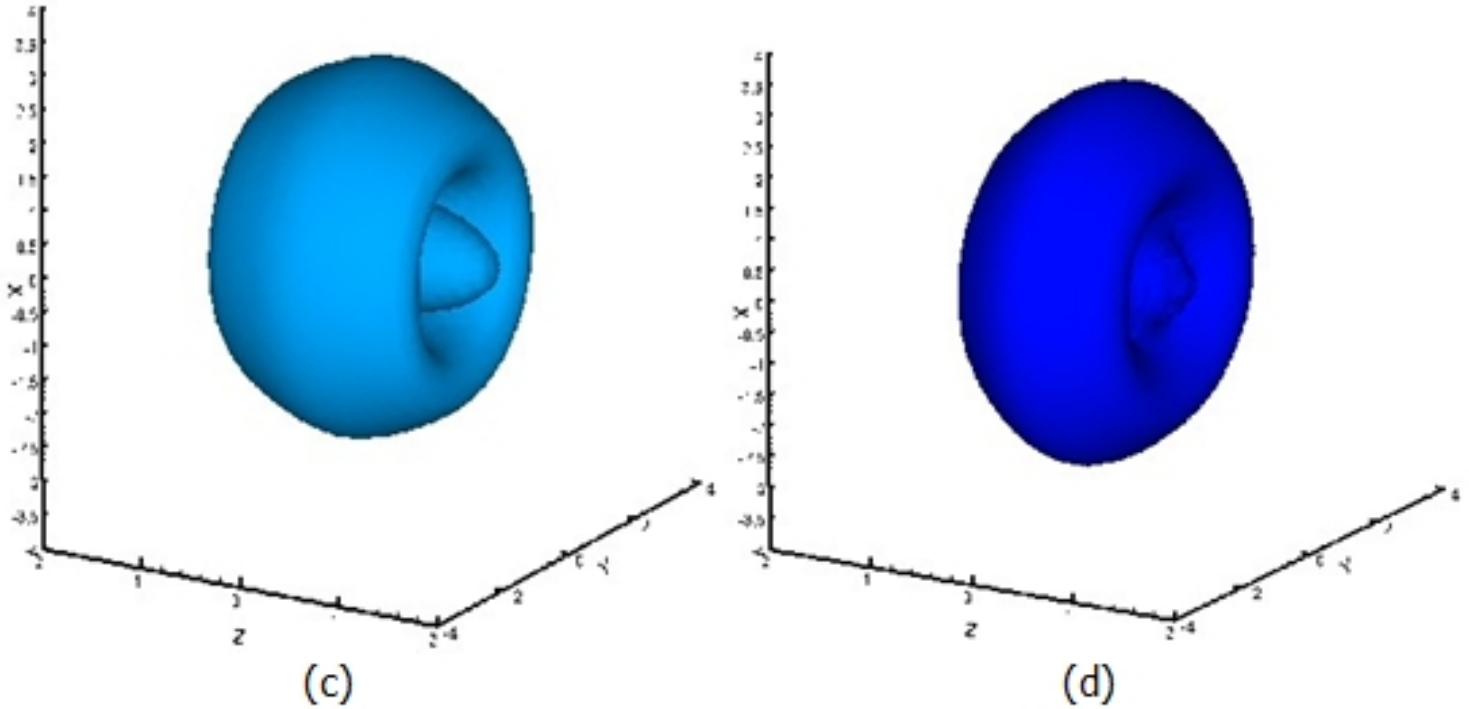


Fig.10. The isosurface plots of density $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at (a) $t = 0.0$, (b) $t = 0.1$, (c) $t = 0.15$, (d) $t = 0.2$ for dipolar BECs with the interaction constant β changing from 103.58 to -569.69 suddenly at time $t = 0$.

Main References

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- D.Y. Hua, X.-G. Li, The finite element method for computing the ground states of the dipolar Bose – Einstein condensates,*Appl. Math. Comput., 234 (2014) 214 – 222.*

Thanks!