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A two-parameter continuation method for computing numerical solutions of spin-1 Bose–Einstein condensates

Y.-S. Wang, C.-S. Chien [*,1]

Department of Computer Science and Information Engineering, Chien Hsin University of Science and Technology, Zhongli 320, Taiwan

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ABSTRACT

We describe a novel two-parameter continuation method combined with a spectral-collocation method (SCM) for computing the ground state and excited-state solutions of spin-1 Bose–Einstein condensates (BEC), where the second kind Chebyshev polynomials are used as the basis functions for the trial function space. To compute the ground state solution of spin-1 BEC, we implement the single parameter continuation algorithm with the chemical potential μ as the continuation parameter, and trace the first solution branch of the Gross–Pitaevskii equations (GPEs). When the curve-tracing is close enough to the target point, where the normalization condition of the wave function is going to be satisfied, we add the magnetic potential λ as the second continuation parameter with the magnetization M as the additional constraint condition. Then we implement the two-parameter continuation algorithm until the target point is reached, and the ground state solution of the GPEs is obtained. The excited state solutions of the GPEs can be treated in a similar way. Some numerical experiments on ^{23}Na and ^{87}Rb are reported. The numerical results on the spin-1 BEC are the same as those reported in [10]. Further numerical experiments on excited-state solutions of spin-1 BEC suffice to show the robustness and efficiency of the proposed two-parameter continuation algorithm.

1. Introduction

Recently, experimental achievements on spin-1 and spin-2 Bose–Einstein condensates (BEC) [1–3] offer new research direction to study various quantum phenomena which do not exist in a single-component BEC. The spinor BEC is achieved in physical experiments when an optical lattice is used to provide equal confinement for all hyperfine states. The theoretic study of spinor BEC can be found in [4,5]. When the temperature is much lower than the critical temperature T_c, the three-component wave function $\Phi(\mathbf{x},t)=(\varphi_1(\mathbf{x},t),\varphi_0(\mathbf{x},t),\varphi_{-1}(\mathbf{x},t))^T$ of a spin-1 BEC is governed by the following coupled Gross–Pitaevskii equations (GPEs) [6–8]:

$$\mathbf{i}\hbar\partial_t\varphi_1(\mathbf{x},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})+(c_0+c_2)\left(|\varphi_1|^2+|\varphi_0|^2\right)+(c_0-c_2)|\varphi_{-1}|^2\right]\varphi_1+c_2\bar{\varphi}_{-1}\varphi_0^2,$$

$$\mathbf{i}\hbar\partial_t\varphi_0(\mathbf{x},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})+(c_0+c_2)\left(|\varphi_1|^2+|\varphi_{-1}|^2\right)+c_0|\varphi_0|^2\right]\varphi_0+2c_2\varphi_{-1}\bar{\varphi}_0\varphi_1,$$

* Corresponding author.
E-mail addresses: cschien@uch.edu.tw, cschien@amath.nchu.edu.tw (C.-S. Chien).

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$$\mathbf{i}\hbar\partial_t\varphi_{-1}(\mathbf{x},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})+(c_0+c_2)\big(|\varphi_{-1}|^2+|\varphi_0|^2\big)+(c_0-c_2)|\varphi_1|^2\right]\varphi_{-1}+c_2\varphi_0^2\bar{\varphi}_1, \tag{1.1}$$

where $\mathbf{x}=(x,y,z)^T\in\mathbf{R}^3$, t is the time, $\hbar$ is the Planck constant, m is the atomic mass, $V(\mathbf{x})=\frac{m}{2}(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2)$ is the external trapping potential with ω_x,ω_y and ω_z being the trap frequencies in the x-, y-, and z-direction, respectively, $c_0=\frac{4\pi\hbar^2}{3m}(a_0+2a_2)$ and $c_2=\frac{4\pi\hbar^2}{3m}(a_2-a_0)$ denote constants of the spin-independent and spin-exchange interaction, respectively, with a_j the s-wave scattering lengths for the channel of total hyperfine spin j $(j=0,2)$. Note that positive and negative c_0 stands for repulsive and attractive interaction, respectively. The spin-exchange interaction c_2 is positive for antiferromagnetic interaction and negative for ferromagnetic interaction. The wave function is normalized according to

$$\|\Phi\|^2:=\int_{\mathbf{R}^3}\big|\Phi(\mathbf{x},t)\big|^2\,d\mathbf{x}=\int_{\mathbf{R}^3}\sum_{l=-1}^{1}\big|\varphi_l(\mathbf{x},t)\big|^2\,d\mathbf{x}:=\sum_{l=-1}^{1}\|\varphi_l\|^2=N, \tag{1.2}$$

where N is the total number of particles in the condensates. By introducing the dimensionless variables and reducing the 3D coupled GPEs (1.1) to 1D coupled GPEs [9,10], we obtain the following coupled GPEs:

$$\begin{aligned}
\mathbf{i}\partial_t\varphi_1(x,t)&=\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+(g_n+g_s)\big(|\varphi_1|^2+|\varphi_0|^2\big)+(g_n-g_s)|\varphi_{-1}|^2\right]\varphi_1+g_s\bar{\varphi}_{-1}\varphi_0^2,\\
\mathbf{i}\partial_t\varphi_0(x,t)&=\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+(g_n+g_s)\big(|\varphi_1|^2+|\varphi_{-1}|^2\big)+g_n|\varphi_0|^2\right]\varphi_0+2g_s\varphi_{-1}\bar{\varphi}_0\varphi_1,\quad x\in\mathbf{R},\\
\mathbf{i}\partial_t\varphi_{-1}(x,t)&=\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+(g_n+g_s)\big(|\varphi_{-1}|^2+|\varphi_0|^2\big)+(g_n-g_s)|\varphi_1|^2\right]\varphi_{-1}+g_s\varphi_0^2\bar{\varphi}_1,
\end{aligned} \tag{1.3}$$

where $g_n=\frac{4\pi N}{3a_s}(a_0+2a_2)$, $g_s=\frac{4\pi N}{3a_s}(a_2-a_0)$ with $a_s=\sqrt{\frac{\hbar}{m\omega_m}}$, $\omega_m=\min\{\omega_x,\omega_y,\omega_z\}$, $V(x)=\frac{1}{2}x^2$. Three important invariants of Eq. (1.3) are the mass (or normalization) of the wave function

$$N\big(\Phi(\cdot,t)\big):=\big\|\Phi(\cdot,t)\big\|^2:=\int_{\mathbf{R}}\sum_{l=-1}^{1}\big|\varphi_l(x,t)\big|^2\,dx\equiv N\big(\Phi(\cdot,0)\big)=1,\quad t>0, \tag{1.4}$$

the magnetization

$$M\big(\Phi(\cdot,t)\big):=\int_{\mathbf{R}}\big[\big|\varphi_1(x,t)\big|^2-\big|\varphi_{-1}(x,t)\big|^2\big]\,dx\equiv M\big(\Phi(\cdot,0)\big)=M,\quad |M|\leqslant 1, \tag{1.5}$$

and the energy per particle

$$\begin{aligned}
E\big(\Phi(\cdot,t)\big):=\int_{\mathbf{R}}\Bigg\{&\sum_{l=-1}^{1}\left[\frac{1}{2}\left|\frac{d}{dx}\varphi_l\right|^2+V(x)|\varphi_l|^2\right]+(g_n-g_s)|\varphi_1|^2|\varphi_{-1}|^2+\frac{g_n}{2}|\varphi_0|^4\\
&+\frac{g_n+g_s}{2}\big[|\varphi_1|^4+|\varphi_{-1}|^4+2|\varphi_0|^2\big(|\varphi_1|^2+|\varphi_{-1}|^2\big)\big]+g_s\big(\bar{\varphi}_{-1}\varphi_0^2\bar{\varphi}_1+\varphi_{-1}\bar{\varphi}_0^2\varphi_1\big)\Bigg\}\,dx,\quad t\geqslant 0.
\end{aligned} \tag{1.6}$$

The ground state of a spin-1 BEC is the lowest energy stationary state which can be obtained from the minimum energy condition of the system (1.6) subject to the constraints (1.4) and (1.5) [9,10]. In this paper, we will be concerned with the stationary state solutions $\Psi(x)=(\psi_1(x),\psi_0(x),\psi_{-1}(x))^T$ of (1.3). In order to solve the minimization problem, we define the Lagrangian

$$L(\Psi,\mu,\lambda):=E(\Psi)-\mu\big(\|\psi_1\|^2+\|\psi_0\|^2+\|\psi_{-1}\|^2-1\big)-\lambda\big(\|\psi_1\|^2-\|\psi_{-1}\|^2-M\big). \tag{1.7}$$

Differentiating (1.7) with respect to ψ_1, ψ_0 and ψ_{-1}, respectively, we obtain the following Euler–Lagrange equation:

$$\begin{aligned}
(\mu+\lambda)\psi_1&=\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+g_n\big(|\psi_1|^2+|\psi_0|^2+|\psi_{-1}|^2\big)\right]\psi_1+g_s\big(|\psi_1|^2+|\psi_0|^2-|\psi_{-1}|^2\big)\psi_1+g_s\psi_{-1}\psi_0^2,\\
\mu\psi_0&=\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+g_n\big(|\psi_1|^2+|\psi_0|^2+|\psi_{-1}|^2\big)\right]\psi_0+g_s\big(|\psi_1|^2+|\psi_{-1}|^2\big)\psi_0+2g_s\psi_{-1}\psi_0\psi_1,\\
(\mu-\lambda)\psi_{-1}&=\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+g_n\big(|\psi_1|^2+|\psi_0|^2+|\psi_{-1}|^2\big)\right]\psi_{-1}+g_s\big(|\psi_0|^2+|\psi_{-1}|^2-|\psi_1|^2\big)\psi_{-1}+g_s\psi_1\psi_0^2,
\end{aligned} \tag{1.8}$$