

A time-splitting spectral scheme for the dynamics of Gross-Pitaevskii-Poisson system

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This paper propose a time-splitting pseudospectral method to investigate the dynamic of ultracold ion-ion quantum plasmas. The wave functions of positive and negative ions are modeled by the Gross-Pitaevskii equations coupled with the Poisson equation for electric potential. The time-splitting scheme on the Gross-Pitaevskii-Poisson system is explicit, unconditionally stable and mass-conserving, which is highly efficient for simulating the coupled system. Numerical examples validate the spectral convergence and unconditional stability, with an X-shape quantum plasma interaction demonstrated.

Index Terms—Time-splitting integrator, Fourier pseudospectral method, Gross-Pitaevskii-Poisson system, ultracold plasmas.

I. INTRODUCTION

ULTRACOLD PLASMAS are a distinct class of plasmas that exhibit strong interparticle interactions from quantum effects, which categorizes them as quantum plasmas and set them apart from classical plasmas such as streamers [1]. They exist under extremely low temperatures [2] and have drawn more attention recently since supercomputers [3] and the nanostructures of semiconductor [4] grow in importance.

Besides the widely studied electron-ion mixtures, a less common type of quantum plasmas consists of a mixture of positive and negative ions, which has been recently studied using the Gross-Pitaevskii-Poisson (GPP) system in [5]. The authors therein adopt the dimensionless symmetric GPP system to describe the coupling of two equal-mass wave functions $\psi_{\pm}$ and electric potential ϕ as

$$i \frac{\partial \psi_+}{\partial t} = -\frac{1}{2} \Delta \psi_+ + \left(g |\psi_+|^2 + G |\psi_-|^2 + q\phi \right) \psi_+, \quad (1)$$

$$i \frac{\partial \psi_-}{\partial t} = -\frac{1}{2} \Delta \psi_- + \left(g |\psi_-|^2 + G |\psi_+|^2 - q\phi \right) \psi_-, \quad (2)$$

$$-\Delta \phi = 4\pi q \left(|\psi_+|^2 - |\psi_-|^2 \right). \quad (3)$$

The subscript “ $\pm$ ” represents the positive ions and negative ions respectively. g and G are the coefficients of contact interactions, and q is the scaled absolute value of charge.

Following [5], we consider a square domain with periodic boundary conditions. Without loss of generality, this domain is denoted as $(0, L)^2$, where L denotes the edge length. Assume the dynamics occurs from time $t = 0$ to $t = T$, and initial conditions for $\psi_{\pm}$ are applied at $t = 0$.

The ground state of the above GPP system has been extensively explored in [5]. However, when it comes to the dynamics of GPP, only one-dimensional results are presented therein, without addressing the numerical methods. Consequently, this paper serves as a complement to [5], which focuses on the detailed and practical numerical scheme and its applications in two dimensions.

II. TIME-SPLITTING SPECTRAL SCHEME

The time-splitting spectral method has been successfully applied to the Schrödinger-Poisson- $X\alpha$ model in [6], which couples the Poisson equation with a single nonlinear Schrödinger equation for electrons. In contrast, our GPP system (1)-(3) features two nonlinear Schrödinger equations, one for positive ions and one for negative ions, incorporating interactions among multiple ions (the G terms in (1)-(2)). Nevertheless, drawing inspiration from the fundamental concept in [6], we are able to adapt and propose the scheme for the GPP system.

The domain is discretized by a uniform mesh with a mesh size of $\Delta x = \Delta y = L/N$, where N is an even integer. Time step is chosen as Δt . Accordingly, $\psi_{\pm jk}^n$ denotes the numerical solutions of $\psi_{\pm}(x_j, y_k, t_n)$, with $x_j = j\Delta x$, $y_k = k\Delta y$, and $t_n = n\Delta t$. Our time-splitting spectral method combines the second-order Strang splitting and the Fourier pseudospectral method. It can be sequentially implemented in four steps. First, we solve linear part of ψ_+ and ψ_- in the phase space as

$$\psi_{\pm jk}^* = \sum_{l,m=-N/2}^{N/2-1} e^{-i(\mu_l^2 + \mu_m^2)\Delta t/4} (\hat{\psi}_{\pm}^n)_{lm} e^{i(\mu_l x_j + \mu_m y_k)}, \quad (4)$$

where

$$\mu_l = \frac{2\pi l}{L}, \quad \hat{\psi}_{lm} = \frac{1}{N^2} \sum_{j,k=0}^{N-1} \psi_{jk} e^{-i(\mu_l x_j + \mu_m y_k)}.$$

Second, the potential ϕ is integrated exactly in the phase space

$$\phi_{jk}^* = \sum_{\substack{l,m=-N/2 \\ |l|+|m|>0}}^{N/2-1} \frac{(|\hat{\psi}_+^n|^2)_{lm} - (|\hat{\psi}_-^n|^2)_{lm}}{(\mu_l^2 + \mu_m^2)/4\pi q} e^{i(\mu_l x_j + \mu_m y_k)}. \quad (5)$$

Third, we integrate the nonlinear part of ψ_+ and ψ_- exactly in the discrete physical space as

$$\psi_{\pm jk}^{**} = e^{-i\Delta t \left(g |\psi_{\pm jk}^*|^2 + G |\psi_{\mp jk}^*|^2 \pm q \phi_{jk}^* \right)} \psi_{\pm jk}^*. \quad (6)$$

Fourth, the linear part of ψ_+ and ψ_- is solved similar to (4)

$$\psi_{\pm jk}^{n+1} = \sum_{l,m=-N/2}^{N/2-1} e^{-i(\mu_l^2 + \mu_m^2)\Delta t/4} (\hat{\psi}_{\pm}^{**})_{lm} e^{i(\mu_l x_j + \mu_m y_k)}. \quad (7)$$

It is noteworthy that, owing to the utilization of the fast Fourier transform, the computational complexity of the entire four steps (4)-(7) is $O(N^2 \log(N))$.

III. PERFORMANCE OF THE SCHEME

This section is dedicated to testing the numerical performance of scheme (4)-(7), with the spatial and temporal convergence examined separately in two subsections. The dimensionless coefficients are set as $g = -1$, $G = 1$ and $q = 1$. The domain is chosen to be $L = 10$, and the dynamics is carried out until $T = 0.5$. Initial values for $\psi_{\pm}$ are

$$\psi_{\pm}(x, y, t = 0) = e^{-((x - \frac{L}{2} \mp 1)^2 + (y - \frac{L}{2})^2)}.$$

A. Spatial accuracy

To show the spatial convergence, we choose a small time step $\Delta t = 0.5/2^{10}$. The results of L^2 errors are summarized in Table I, where the spectral convergence is manifestly observed.

TABLE I
 L^2 ERROR AND ORDER OF CONVERGENCE IN SPACE.

N	2^2	2^3	2^4	2^5
$\ \psi_+ - \psi_+^{\text{ref}}\ _2$	1.20×10^0	7.77×10^{-1}	2.30×10^{-2}	5.23×10^{-6}
order	—	0.63	5.08	12.10
$\ \psi_- - \psi_-^{\text{ref}}\ _2$	1.36×10^0	9.10×10^{-1}	4.51×10^{-2}	4.71×10^{-6}
order	—	0.59	4.33	13.23
computational time (ms)	1.30×10^1	1.65×10^1	4.20×10^1	1.26×10^2

$\psi_{\pm}^{\text{ref}}$ are computed by a fine mesh with $N = 2^{10}$.

B. Stability and temporal accuracy

We select a fine mesh with $\Delta x = \Delta y = L/2^{10}$ to demonstrate the temporal properties. The L^2 errors are reported in Table II, where second-order temporal convergence is readily observable. Moreover, it also illustrates the unconditional stability, as the scheme remains stable even when $\Delta t/\Delta x = 2^8$.

TABLE II
 L^2 ERROR AND ORDER OF CONVERGENCE IN TIME.

Δt	$1/2^3$	$1/2^4$	$1/2^5$	$1/2^6$
$\ \psi_+ - \psi_+^{\text{ref}}\ _2$	9.19×10^{-3}	2.29×10^{-3}	5.71×10^{-4}	1.43×10^{-4}
order	—	2.01	2.00	2.00
$\ \psi_- - \psi_-^{\text{ref}}\ _2$	9.19×10^{-3}	2.29×10^{-3}	5.71×10^{-4}	1.43×10^{-4}
order	—	2.01	2.00	2.00

$\psi_{\pm}^{\text{ref}}$ are computed by a small time step $\Delta t = 1/2^{11}$.

IV. APPLICATION

In this section, we present an example of the interaction of ultracold plasmas. The coefficients are adopted from [5] as $g = -1$, $G = 0.9$ and $q = 0.3$. The domain is selected as $L = 20$ with mesh size $\Delta x = \Delta y = L/2^{10}$. A time step of

$\Delta t = 1/2^9$ is chosen, and the initial values follow an X-shape as $\psi_{\pm}(x, y, t = 0) =$

$$e^{-((x - \frac{L}{2} - 2)^2 + (y - \frac{L}{2} \mp 2)^2)} + e^{-((x - \frac{L}{2} + 2)^2 + (y - \frac{L}{2} \pm 2)^2)}.$$

Figure 1 shows the dynamical interaction. On the one hand, the Coulomb coupling from the Poisson equation induces the attraction between ions of different polarities, manifesting the plasma properties. On the other hand, the wave propagation and attractive contact self-interaction come from quantum effects.

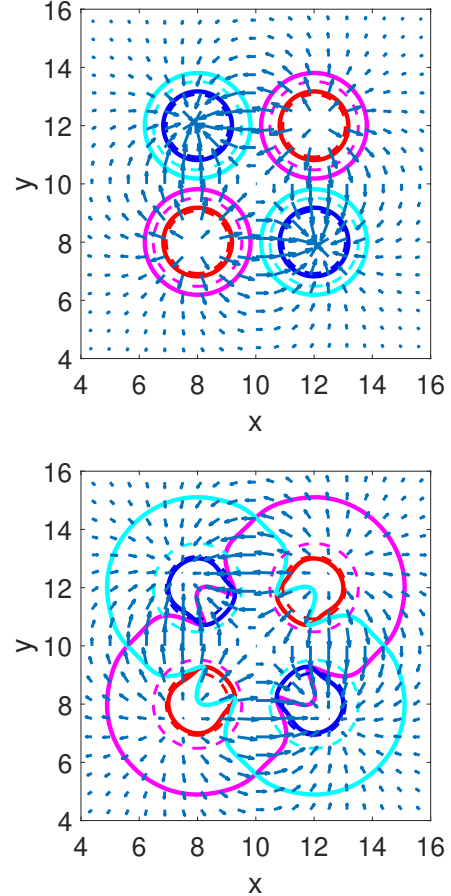


Fig. 1. X-shape interaction of ultracold plasmas at $t = 0.4$ (top) and 1.4 (bottom): Red / light red solid lines for $|\psi_+|^2 = 10^{-1}/10^{-2}$; blue / light blue solid lines for $|\psi_-|^2 = 10^{-1}/10^{-2}$; dashed lines for initial reference; arrows for electric field.

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