

# Bifurcation between 2-component and 3-component ground states of spin-1 Bose-Einstein condensates in uniform magnetic fields\*

Liren Lin<sup>†,1</sup> and I-Liang Chern<sup>‡,1,2,3</sup>

<sup>1</sup>*Department of Mathematics, National Taiwan University, Taipei 106, Taiwan*

<sup>2</sup>*Department of Applied Mathematics, National Chiao Tung University, Hsinchu 300, Taiwan*

<sup>3</sup>*Center of Mathematical Modeling and Scientific Computing, Hsinchu 300, Taiwan*

## Abstract

We study antiferromagnetic spin-1 Bose-Einstein condensates under external uniform magnetic fields. The bifurcation between two-component and three-component regimes of ground states with respect to the magnetization  $M$  and the quadratic Zeeman effect  $q$  is justified. The proof is based on the technique of “mass redistribution” introduced in the authors previous work, which gives interesting inequalities and equalities satisfied by ground states. Some open problems arising naturally from our investigation are also discussed in the end.

## 1 Introduction

Ever since the first realization of Bose-Einstein condensation (BEC) in 1995 [1, 4, 9], it has drawn great attentions of physicists as well as mathematicians. In early experiments, the atoms were confined in magnetic traps, in which the spin degrees of freedom are frozen. By the mean-field approximation, such a system is then described by a scalar wave function, which satisfies the Gross-Pitaevskii (GP) equation [8, 12, 24]. In contrast, in an optically trapped atomic BEC, all its hyperfine spin states can be active simultaneously, and a spin- $F$  BEC has to be described by a  $(2F + 1)$ -component vector function  $\Psi = (\psi_F, \psi_{F-1}, \dots, \psi_{-F})^T$ . Such spinor BEC was first realized in a gas of spin-1  $^{23}\text{Na}$  atoms in 1998 by the MIT group [25, 26, 22, 3, 11], and soon after that its theory was developed independently by several researchers [23, 13, 16]. Since then, it

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\*This work was partially supported by the National Science Council of the Republic of China under Contract Nos. 99-2115-M-002-003-MY3.

<sup>†</sup>b90201033@ntu.edu.tw

<sup>‡</sup>chern@math.ntu.edu.tw

has also become a subject of intensive studies, both theoretically and numerically. On the other hand, although there are already many mathematical investigations of BEC systems with multiple (even general  $N$ ) components [21], the specific structures of spinor BEC are not paid full attentions to by mathematicians. In this paper we consider the mean field ground states of spin-1 BEC. Before introducing the problems and goals to be studied, we shall describe the mathematical model first.

As mentioned above, in the mean field approximation a spin-1 BEC is described by a three-component complex-valued  $\Psi = (\psi_1, \psi_0, \psi_{-1})^T$ . Since we will only be interested in ground states, we consider  $\Psi$  as a function of the space variable  $x \in \mathbb{R}^3$  and is independent of time. Under a uniform magnetic field, the system is described by the energy functional [26, 28, 15]

$$E[\Psi] = \int_{\mathbb{R}^3} \left\{ \sum_j |\nabla\psi_j|^2 + V(x)|\Psi|^2 + \beta_n|\Psi|^4 + \beta_s|\Psi^*F\Psi|^2 + p(|\psi_1|^2 - |\psi_{-1}|^2) + q(|\psi_1|^2 + |\psi_{-1}|^2) \right\} dx,$$

where  $V(x)$  is a real-valued function,  $\beta_n, \beta_s, p, q$  are real constants, and  $F = (F_x, F_y, F_z)$  is the triple of spin-1 Pauli matrices, which are given by

$$F_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad F_y = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad F_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Thus  $\Psi^*F\Psi$  denotes the vector  $(\Psi^*F_x\Psi, \Psi^*F_y\Psi, \Psi^*F_z\Psi)$ . The notation  $|\Psi|$  denotes the Euclidean length  $(\sum_j |\psi_j|^2)^{1/2}$ , and similarly for  $|\nabla\psi_j|$  and  $|\Psi^*F\Psi|$ . We remark that here the coefficients of the terms of  $E[\Psi]$  are normalized and are different from those used in the literature for simplicity. Physically,  $V(x)$  represents a state-independent trap potential, the terms with coefficients  $\beta_n$  and  $\beta_s$  describe the collisions of the atoms, and  $p, q$  give the linear and quadratic Zeeman effects, which can be tuned by changing the magnitude of the applied magnetic field. The number of atoms  $\mathcal{N}[\Psi]$  and the total magnetization  $\mathcal{M}[\Psi]$  of the system are given by

$$\mathcal{N}[\Psi] = \int_{\mathbb{R}^3} |\Psi|^2, \quad \mathcal{M}[\Psi] = \int_{\mathbb{R}^3} (|\psi_1|^2 - |\psi_{-1}|^2).$$

And a ground state is a minimizer of  $E$  under fixed  $\mathcal{N}$  and  $\mathcal{M}$ . Thus it's a variational problem with two constraints. By normalization, we shall assume  $\mathcal{N}[\Psi] = 1$ , and  $\mathcal{M}[\Psi] = M$  for some constant  $M$ . Note that  $|\mathcal{M}[\Psi]| \leq \mathcal{N}[\Psi]$  for every state  $\Psi$ , so we must have  $|M| \leq 1$ . Due to the symmetry of the roles of  $\psi_1$  and  $\psi_{-1}$ , we will only consider  $0 \leq M \leq 1$ . We will consider the following setting for our model, which is quite general for the interested phenomenon in this work.

(A1)  $V \in L_{loc}^\infty$ , and  $V(x)$  tends to infinity uniformly as  $x$  tends to infinity. Precisely

$$\lim_{R \rightarrow \infty} (\text{ess inf}_{|x| \geq R} V(x)) = \infty.$$

In particular  $V$  is bounded from below.

(A2)  $\beta_n > 0$  (repulsive) and  $\beta_s > 0$  (antiferromagnetic).

(A3)  $q \geq 0$ .

Assumption (A1) will guarantee that  $V(x)$  traps the repulsive system in a localized region, which is essential for the existence of ground states. Besides these three assumptions, also note that due to the conservations of  $\mathcal{N}$  and  $\mathcal{M}$ , ground states are not changed by shifting the values of  $V(x)$  and  $p$  by any constants, and hence we shall also assume for simplicity

(A4)  $V \geq 0$  and  $p = 0$ .

This work is mainly motivated by the following observation: For fixed  $0 < M < 1$ , as  $q$  increases from zero, the ground state  $\Psi$  undergoes a bifurcation from  $\psi_0 = 0$  to  $\psi_0 \neq 0$  at a critical point  $q_c(M)$ , hence from a two-component (2C) profile to a three-component (3C) one. This phenomenon has been known for many years from numerical simulations [28, 19] (A clear diagram showing the 2C regime and the 3C regime with respect to  $M$  and  $q$  is provided by Fig. 5 in [19].), and was recently observed experimentally [14]. However, there seems to be no rigorous mathematical justification so far. In theoretical explanations by physicists, some simplified assumptions such as uniformity (assuming  $\Psi$  is a constant vector) or single-mode approximation (assuming the components of  $\Psi$  are proportional to each other) are made, which have no sufficient reason for being satisfactory demonstrations. In [20], the authors found a principle which says that after a redistribution of the masses between different components, the kinetic energy will decrease. Using this fact, we successfully proved, among other things, the vanishing of  $\psi_0$  of the ground state at  $q = 0$  (i.e. no external magnetic field). In the present work, we will show that the bifurcation phenomenon can also be deduced from the same principle, while not as obviously as before. Some basic properties about ground states have to be established first. It's interesting that many of the facts addressed in this paper can also be derived by using the idea of mass redistribution.

The outline of the paper is as follows. Section 2 contains the basics of the model. We first introduce a well-known reduction by which one can simply study the amplitudes of the components of  $\Psi$ . Then, after defining some notations in Section 2.1, the most fundamental properties such as existence, regularity and maximum principle are given in Section 2.2. In Section 3 we recap the idea of mass redistribution and, with the aid of it, prove some more useful facts about ground states: the continuity and monotonicity of ground-state energy with respect to  $M$  and  $q$ , the fact  $|\psi_1| \geq |\psi_{-1}|$ , and the exponential

decaying of ground states as  $|x| \rightarrow \infty$ . In Section 4 we introduce an idea of perturbation by redistribution, which gives rise to some inequalities and equalities satisfied by ground states. In Section 5.1 the bifurcation phenomenon is justified by using the inequalities obtained in Section 4. Some approximations and characterizations of the bifurcation point induced by our proof are given in Section 5.2. In Section 6 we discuss three open problems naturally arising from this work.

## 2 Preliminaries

### 2.1 Reductions and notations

We use  $\mathbb{B}$  to denote the function space  $(H^1(\mathbb{R}^3) \cap L_V^2(\mathbb{R}^3) \cap L^4(\mathbb{R}^3))^3$ , where  $L_V^2$  is the  $V$ -weighted  $L^2$  space: A measurable function  $f$  is in  $L_V^2(\mathbb{R}^3)$  if  $\|f\|_{L_V^2}^2 := \int |f|^2 V < \infty$ . (When the domain of an integration is not specified, it's understood to be  $\mathbb{R}^3$ .)  $\mathbb{B}$  is a Banach space endowed with the following norm:

$$\|\Psi\|^2 = \int \left\{ |\Psi|^2 + \sum_j |\nabla \psi_j|^2 + V|\Psi|^2 + |\Psi|^4 \right\}.$$

Given  $\Psi = (\psi_1, \psi_0, \psi_{-1}) \in \mathbb{B}$ . Let  $\psi_j = |\psi_j|e^{i\theta_j}$  be the polar form of the  $j$ -th component. Then we have (remember we have assumed  $p = 0$ )

$$\begin{aligned} E[\Psi] = \int_{\mathbb{R}^3} \left\{ \sum_j |\nabla \psi_j|^2 + V(x)|\Psi|^2 + \beta_n |\Psi|^4 \right. \\ \left. + 2\beta_s |\psi_0|^2 \left[ |\psi_1|^2 + |\psi_{-1}|^2 + 2|\psi_1||\psi_{-1}| \cos(\theta_1 - 2\theta_0 + \theta_{-1}) \right] \right. \\ \left. + \beta_s (|\psi_1|^2 - |\psi_{-1}|^2)^2 + q(|\psi_1|^2 + |\psi_{-1}|^2) \right\} dx. \end{aligned}$$

Since  $|\nabla \psi_j| \geq |\nabla |\psi_j||$  by the convexity inequality for gradients (see e.g. [17], 7.8), we find  $E[\Psi] \geq \mathcal{E}(|\psi_1|, |\psi_0|, |\psi_{-1}|)$ , where

$$\begin{aligned} \mathcal{E}[\mathbf{u}] := \int_{\mathbb{R}^3} \left\{ \sum_j |\nabla u_j|^2 + V(x)|\mathbf{u}|^2 + \beta_n |\mathbf{u}|^4 \right. \\ \left. + \beta_s \left[ 2u_0^2 (u_1 - u_{-1})^2 + (u_1^2 - u_{-1}^2)^2 \right] + q(u_1^2 + u_{-1}^2) \right\} dx \end{aligned}$$

for nonnegative triples  $\mathbf{u} = (u_1, u_0, u_{-1}) \in \mathbb{B}$ . The equality holds if the  $\theta_j$ 's are constants and satisfy

$$\cos(\theta_1 - 2\theta_0 + \theta_{-1}) = -1. \tag{2.1}$$

Also, note that the conservations of  $\mathcal{N}$  and  $\mathcal{M}$  are constraints on  $|\psi_j|$  and have nothing to do with the phases. These observations lead us to consider the following variational problem:

$$(*) \quad \begin{aligned} & \text{Minimizing } \mathcal{E} \text{ over the family of nonnegative triples} \\ & \mathbf{u} \in \mathbb{B} \text{ satisfying } \mathcal{N}[\mathbf{u}] = 1 \text{ and } \mathcal{M}[\mathbf{u}] = M. \end{aligned}$$

It's not hard to prove that if  $\Psi$  is a ground state,  $\mathbf{u} = (|\psi_1|, |\psi_0|, |\psi_{-1}|)$  is a solution of (\*). Conversely, if  $\mathbf{u} = (u_1, u_0, u_{-1})$  is a solution of (\*), then  $\Psi = (\psi_1, \psi_0, \psi_{-1})$  defined by  $\psi_j = u_j e^{i\theta_j}$  for any choice of constants  $\theta_j$  satisfying (2.1) is a ground state. As a consequence, to understand the bifurcation phenomenon introduced in Section 1, it suffices to study (\*). We will do so in the rest of this paper and no longer consider  $E$ . To facilitate later discussion we introduce some notations in the following.

First let's make the rule that when a boldface letter, possibly with a superscript, is used to denote an element in  $\mathbb{B}$ , its components are denoted by the same letter in normal font with indices 1, 0,  $-1$ . For example  $\mathbf{u}$  denotes  $(u_1, u_0, u_{-1})$  as before, and similarly  $\mathbf{v}$  denotes  $(v_1, v_0, v_{-1})$ ,  $\mathbf{w}^k$  denotes  $(w_1^k, w_0^k, w_{-1}^k)$ , etc. We say a sequence in  $\mathbb{B}$  converges weakly if it converges weakly in  $(H^1(\mathbb{R}^3))^3$ , in  $(L_V^2(\mathbb{R}^3))^3$ , and in  $(L^4(\mathbb{R}^3))^3$ . Due to the reflexivity of  $H^1$ ,  $L_V^2$  and  $L^4$ , every bounded sequence in  $\mathbb{B}$  has a weakly convergent subsequence. Let

$$\mathbb{B}_+ = \{\mathbf{u} \in \mathbb{B} \mid u_j \geq 0 \text{ for each } j\}.$$

We have the following fact.

**Lemma 2.1.**  $\mathbb{B}_+$  is a weakly closed subset of  $\mathbb{B}$ .

*Proof.* Let  $\{\mathbf{u}^k\}$  be a sequence in  $\mathbb{B}_+$  which weakly converges to some  $\mathbf{u}^\infty \in \mathbb{B}$ . We need to prove  $u_j^\infty \geq 0$  for each  $j$ . Let  $H^+ = \{\mathbf{u} \in (H^1(\mathbb{R}^3))^3 \mid u_j \geq 0 \text{ for each } j\}$ . Note that  $\{\mathbf{u}^k\}$  is also a sequence in  $H^+$  weakly converging to  $\mathbf{u}^\infty$  in  $(H^1(\mathbb{R}^3))^3$ . Since  $H^+$  is a convex and closed subset of  $(H^1(\mathbb{R}^3))^3$ ,  $H^+$  is a weakly closed subset of  $(H^1(\mathbb{R}^3))^3$  by Mazur's theorem (see e.g. [5], Theorem 3.7). Thus  $\mathbf{u}^\infty \in H^+$ , that is  $u_j^\infty \geq 0$  for each  $j$ .  $\square$

The admissible class on which we are going to minimize  $\mathcal{E}$  is

$$\mathbb{A} = \{\mathbf{u} \in \mathbb{B}_+ \mid \mathcal{N}[\mathbf{u}] = 1 \text{ and } \mathcal{M}[\mathbf{u}] = M\}.$$

The ground-state energy will be denoted by  $E_g$ , that is

$$E_g = \inf_{\mathbf{v} \in \mathbb{A}} \mathcal{E}[\mathbf{v}].$$

And the set of minimizers is

$$\mathbb{G} = \{\mathbf{u} \in \mathbb{A} \mid \mathcal{E}[\mathbf{u}] = E_g\}.$$

For convenience, we will also frequently refer to elements in  $\mathbb{G}$  as ground states. When  $M$  and  $q$  are regarded as variable parameters, we shall write  $\mathbb{A}_M$ ,  $E_g(M, q)$ , and  $\mathbb{G}_{M,q}$  to specify their values explicitly. Throughout this paper other parameters of our model are considered to be fixed and satisfy (A1) – (A4). Finally, we will use  $H(\mathbf{u})$  to denote the integrand of  $\mathcal{E}[\mathbf{u}]$ , i.e.  $\mathcal{E}[\mathbf{u}] = \int H(\mathbf{u})$ . For convenience we write

$$H(\mathbf{u}) = H_{kin}(\mathbf{u}) + H_{pot}(\mathbf{u}) + H_n(\mathbf{u}) + H_s(\mathbf{u}) + H_{Zee}(\mathbf{u}),$$

where  $H_{kin}(\mathbf{u}) = |\nabla \mathbf{u}|^2$ ,  $H_{pot}(\mathbf{u}) = V|\mathbf{u}|^2$ ,  $H_n(\mathbf{u})$  and  $H_s(\mathbf{u})$  represent the terms with coefficients  $\beta_n$  and  $\beta_s$  respectively, and  $H_{Zee}(\mathbf{u})$  represents the term with coefficient  $q$ . Accordingly, we also use  $\mathcal{E}_{kin}$ ,  $\mathcal{E}_{pot}$ , etc. to denote the corresponding parts of  $\mathcal{E}$ .

## 2.2 Basic properties

In many aspects our three-component system can be regarded as a generalization of the one-component BEC model studied in [18] (though the main interests in this paper are different from theirs). The most fundamental properties about the one-component model (Theorem 2.1 of [18]) hold naturally for our three-component system (with however a remarkable exception: uniqueness. See Remark 2.2 and Section 6.1). We summarize them in the following theorem.

**Theorem 2.2.**  $\mathbb{G} \neq \emptyset$ , i.e. there does exist a ground state. Let  $\mathbf{u} \in \mathbb{G}$ , then  $\mathbf{u}$  is at least once continuously differentiable, and  $\mathbf{u}$  satisfies the following Euler-Lagrange system in the sense of distribution:

$$(\mu + \lambda)u_1 = \mathcal{L}u_1 + 2\beta_s [u_0^2(u_1 - u_{-1}) + u_1(u_1^2 - u_{-1}^2)] + qu_1 \quad (2.2a)$$

$$\mu u_0 = \mathcal{L}u_0 + 2\beta_s u_0(u_1 - u_{-1})^2 \quad (2.2b)$$

$$(\mu - \lambda)u_{-1} = \mathcal{L}u_{-1} + 2\beta_s [u_0^2(u_{-1} - u_1) + u_{-1}(u_{-1}^2 - u_1^2)] + qu_{-1}, \quad (2.2c)$$

where  $\mathcal{L} = -\Delta + V + 2\beta_n|\mathbf{u}|^2$ , and  $\lambda, \mu$  are Lagrange multipliers arising from the constraints  $\mathcal{N}[\mathbf{u}] = 1$  and  $\mathcal{M}[\mathbf{u}] = M$  respectively. Furthermore, for each  $u_j$ , either  $u_j \equiv 0$  or  $u_j > 0$  on all of  $\mathbb{R}^3$ .

We give some remarks. First, due to the repulsive assumption (A2), the existence result can be proved by the standard direct method in the calculus of variations, in which one tries to show that a minimizing sequence has a subsequence that weakly converges to an element in  $\mathbb{G}$ . The only difference from a typical situation is that here the system is on the whole space but not a bounded domain. As a result, we do not have compact embedding  $H^1 \hookrightarrow L^2$  to guarantee that the weak limit is still in the same admissible class. Instead, we should use the assumption (A1), which implies that most part of  $\mathbf{u}$  is really contained in bounded domains, on which compact embedding applies. A precise argument can be given almost the same as in Lemma A.2 of [18] (see also [2, 6]). Nevertheless, besides the conclusion of existence, some observations from the proof will

also be needed later. We give them in Lemma 2.3 below. The most important point is that we actually have strong convergence but not only weak convergence for the subsequence of the minimizing sequence. This holds for our model since all the terms (namely  $H_{kin}$ ,  $H_{pot}$ , etc.) of  $H$  are nonnegative. For convenience we give the proof in the appendix.

**Lemma 2.3.** *Let  $\{\mathbf{u}^n\}$  be a sequence in  $\mathbb{B}_+$ . Suppose  $\mathcal{N}[\mathbf{u}^n] \rightarrow 1$ ,  $\mathcal{M}[\mathbf{u}^n] \rightarrow M$ , and  $\mathcal{E}[\mathbf{u}^n]$  is uniformly bounded in  $n$ , then  $\{\mathbf{u}^n\}$  has a subsequence  $\{\mathbf{u}^{n(k)}\}_{k=1}^\infty$  converging weakly to some  $\mathbf{u}^\infty \in \mathbb{A}$ , which satisfies  $\mathcal{E}[\mathbf{u}^\infty] \leq \liminf_{k \rightarrow \infty} \mathcal{E}[\mathbf{u}^{n(k)}]$ . If we assume further that  $\mathcal{E}[\mathbf{u}^n] \rightarrow E_g$ , then  $\mathbf{u}^\infty \in \mathbb{G}$ , and  $\mathbf{u}^{n(k)} \rightarrow \mathbf{u}^\infty$  in the norm of  $\mathbb{B}$ .*

Next, for the remaining assertions of Theorem 2.2: The Euler-Lagrange system (2.2) is called a time-independent Gross-Pitaevskii system (GP system for short). We remark that by definition (2.2) holds in the sense of distribution, while by approximation we see it's also valid when tested by elements in  $\mathbb{B}$ . In fact,  $\mathcal{E}, \mathcal{N}, \mathcal{M}$  are continuously differentiable functions on  $\mathbb{B}$ , and (2.2) is exactly

$$\frac{\mu}{2} \mathcal{N}'[\mathbf{u}] + \frac{\lambda}{2} \mathcal{M}'[\mathbf{u}] = \frac{1}{2} \mathcal{E}'[\mathbf{u}], \quad (2.3)$$

where  $'$  denotes Fréchet derivative. We omit the routine verification of this fact. Once (2.2) is obtained, that  $\mathbf{u} \in \mathbb{G}$  is continuously differentiable follows standard regularity theorem (e.g. [17], 10.2). And the strict positivity of a nonvanishing component can be obtained by the strong maximum principle (see e.g. [10], Theorem 8.19). We will use these two facts tacitly to avoid repeatedly referring to Theorem 2.2.

**Corollary 2.4.** *Let  $\mathbf{u} \in \mathbb{G}$ . If  $0 < M < 1$ , then  $u_j \neq 0$  for  $j = 1, -1$ .*

*Proof.* Since  $\int (u_1^2 - u_{-1}^2) = M > 0$ ,  $u_1 \neq 0$ , and hence  $u_1 > 0$ . To prove  $u_{-1} \neq 0$ , assume otherwise, then (2.2c) gives  $u_0^2 u_1 = 0$ , and so  $u_0 = 0$ . Thus among the three components only  $u_1 \neq 0$ , which implies  $M = 1$ , contradicting to our assumption.  $\square$

*Remark 2.1.* The assumption  $0 < M < 1$  is necessary. If  $M = 1$ , it's obvious that only  $u_1 \neq 0$ . For  $M = 0$ , see Proposition 3.7 and the remark following it.

As is mentioned in the introduction, we will investigate whether  $u_0$  vanishes or not, as a property depending on the values of  $M$  and  $q$ . Let's here use  $\mathbb{B}_+^{two}$  to denote the class of all  $\mathbf{u} \in \mathbb{B}_+$  such that  $u_0 = 0$ , and let  $\mathbb{A}^{two} = \mathbb{A} \cap \mathbb{B}_+^{two}$ . Note that for  $\mathbf{u} \in \mathbb{A}^{two}$  the constraints are

$$\int u_1^2 = \frac{1+M}{2} \quad \text{and} \quad \int u_{-1}^2 = \frac{1-M}{2}.$$

Then we define

$$\mathbb{G}^{two} = \left\{ \mathbf{u} \in \mathbb{A}^{two} \mid \mathcal{E}[\mathbf{u}] = \inf_{\mathbf{v} \in \mathbb{A}^{two}} \mathcal{E}[\mathbf{v}] \right\}.$$

Obviously, if  $\mathbf{u} \in \mathbb{G}$  is such that  $u_0 = 0$ , then  $\mathbf{u} \in \mathbb{G}^{two}$ .

The assertions in Theorem 2.2 for  $\mathbb{G}$  (existence, regularity, and positivity of a non-vanishing component) also hold for  $\mathbb{G}^{two}$ . The Euler-Lagrange system for  $\mathbf{u} \in \mathbb{G}^{two}$  just consists of (2.2a) and (2.2c) with  $u_0 = 0$ . A particular feature of the two-component system is the following convexity property.

**Lemma 2.5.** *Given  $\mathbf{u}, \mathbf{v} \in \mathbb{B}_+^{two}$ . Let  $\mathbf{w} \in \mathbb{B}_+^{two}$  be defined by  $w_j^2 = (u_j^2 + v_j^2)/2$  for  $j = 1, -1$ , then  $\mathcal{E}[\mathbf{w}] \leq (\mathcal{E}[\mathbf{u}] + \mathcal{E}[\mathbf{v}])/2$ .*

*Proof.* Let  $D = (\mathcal{E}[\mathbf{u}] + \mathcal{E}[\mathbf{v}])/2 - \mathcal{E}[\mathbf{w}]$ , then  $D = D_{kin} + D_n + D_s$ , where

$$D_{kin} = \frac{\mathcal{E}_{kin}[\mathbf{u}] + \mathcal{E}_{kin}[\mathbf{v}]}{2} - \mathcal{E}_{kin}[\mathbf{w}] = \int \sum_{j=1,-1} \left( \frac{|\nabla u_j|^2 + |\nabla v_j|^2}{2} - |\nabla w_j|^2 \right),$$

which is nonnegative by the convexity inequality for gradients. Also,

$$D_n = \frac{\mathcal{E}_n[\mathbf{u}] + \mathcal{E}_n[\mathbf{v}]}{2} - \mathcal{E}_n[\mathbf{w}] = \frac{\beta_n}{4} \int (|\mathbf{u}|^2 - |\mathbf{v}|^2)^2 \geq 0,$$

and

$$D_s = \frac{\mathcal{E}_s[\mathbf{u}] + \mathcal{E}_s[\mathbf{v}]}{2} - \mathcal{E}_s[\mathbf{w}] = \frac{\beta_s}{4} \int (u_1^2 - u_{-1}^2 - v_1^2 + v_{-1}^2)^2 \geq 0,$$

as are easily checked. Thus  $D \geq 0$ , which is what we want to show.  $\square$

From this convexity property we obtain the following uniqueness result.

**Theorem 2.6.** *There exists exactly one element in  $\mathbb{G}^{two}$ .*

*Proof.* In the above proof, if we further assume that  $\mathbf{u}$  and  $\mathbf{v}$  are in  $\mathbb{G}^{two}$ , then we have  $\mathbf{w} \in \mathbb{A}^{two}$ , and hence  $\mathcal{E}[\mathbf{w}] \geq (\mathcal{E}[\mathbf{u}] + \mathcal{E}[\mathbf{v}])/2$ . Thus we must have  $D_{kin} = D_n = D_s = 0$ . From  $D_n = 0$  and  $D_s = 0$  we conclude that  $\mathbf{u} = \mathbf{v}$ .  $\square$

Besides uniqueness, another particular feature for  $\mathbb{G}^{two}$  is that the element in it doesn't depend on the value of  $q$ . This is due to the fact that  $\mathcal{E}_{Zee}$  equals the constant  $q$  on  $\mathbb{A}^{two}$  and plays no role in the minimization of  $\mathcal{E}$ . In the following we will use  $\mathbf{z}^M$  to denote this two-component ground state corresponding to magnetization  $M$ .

*Remark 2.2.* The above proof of uniqueness by the convexity property of Lemma 2.5 is a standard one. Unfortunately, we cannot obtain uniqueness of  $\mathbf{u} \in \mathbb{G}$  by the same method, at least not in an obvious way. The problem comes from the term  $2\beta_s u_0^2 (u_1 - u_{-1})^2$  in  $H_s(\mathbf{u})$ . In fact, it is shown in [20] that uniqueness fails for  $M = q = 0$ . On the other hand, for  $M = 1$ , or  $M = 0$  and  $q > 0$ , the ground state reduces to a single component (cf. Remark 2.1), and uniqueness can also be obtained by the convexity property. (And obviously such one-component ground states are also independent of  $q$ .) Except for these degenerate situations, however, we do not know how to prove or disprove uniqueness. See Section 6.1 for more discussion on the difficulty of proving uniqueness.

### 3 Redistribution and Some Further Properties

In this section we establish some basic results that will be useful. We'll frequently use the method of “mass redistribution”, or simply redistribution, introduced in [20]. For convenience we recap the idea below.

Let  $f_1, f_2, \dots, f_n, g_1, g_2, \dots, g_m$  be nonnegative functions in  $H^1(\Omega)$ , where  $\Omega$  is a domain in  $\mathbb{R}^N$ , and  $n, m$  are arbitrary finite numbers. Then we say  $(g_1, \dots, g_m)$  is a redistribution of  $(f_1, \dots, f_n)$  if  $g_i^2 = \sum_{j=1}^n a_{ij} f_j^2$  for each  $i = 1, \dots, m$ , where the coefficients  $a_{ij}$  are nonnegative constants satisfying  $\sum_{i=1}^m a_{ij} = 1$  for each  $j = 1, \dots, n$ . If this is the case, it's easily seen that

$$\sum_{i=1}^m g_i^2 = \sum_{j=1}^n f_j^2. \quad (3.1)$$

Moreover, we can prove

$$\sum_{i=1}^m |\nabla g_i|^2 \leq \sum_{j=1}^n |\nabla f_j|^2. \quad (3.2)$$

In the remaining of this paper we shall use the notations  $\mathbb{A}_M, \mathbb{G}_{M,q}$  and  $E_g(M, q)$  to specify the values of  $M$  and  $q$  explicitly. Redistribution provides a simple and concrete way to variate an element in  $\mathbb{A}_M$  into another element, in the same space or in another  $\mathbb{A}_{M'}$ . Indeed, from (3.1), if  $\mathbf{v}$  is a redistribution of some  $\mathbf{u} \in \mathbb{A}_M$ , then  $|\mathbf{v}| = |\mathbf{u}|$ , so the first constraint  $\mathcal{N}[\mathbf{v}] = 1$  is satisfied automatically, and one needs only to take care of the second constraint. Also, the two relations (3.1) and (3.2) of redistribution enable us to easily compare  $\mathcal{E}[\mathbf{u}]$  with  $\mathcal{E}[\mathbf{v}]$ . Precisely, we have  $\mathcal{E}_{pot}[\mathbf{v}] = \mathcal{E}_{pot}[\mathbf{u}]$  and  $\mathcal{E}_n[\mathbf{v}] = \mathcal{E}_n[\mathbf{u}]$  from (3.1), and  $\mathcal{E}_{kin}[\mathbf{v}] \leq \mathcal{E}_{kin}[\mathbf{u}]$  from (3.2). As will be seen, these features make it easy to deduce some facts by using redistribution, which might otherwise be harder to obtain or need more elaboration.

#### 3.1 Continuity and monotonicity of $E_g(M, q)$

In this subsection we prove that  $E_g(M, q)$  is a continuous function, and is increasing in each variable. Since the two variables are of quite different natures, we treat them separately: Consider  $E_g(\cdot, q)$  for fixed  $q$ , and consider  $E_g(M, \cdot)$  for fixed  $M$ .

##### 3.1.1 $E_g$ as a function of $M$

In the following we fix a  $q \geq 0$  and consider  $E_g(\cdot, q)$ . The proof of continuity will rely on the monotonicity, and hence we prove the latter first. For this we need the following lemma.

**Lemma 3.1.**  $\mathcal{E}$  is bounded on  $\cup_{0 \leq M \leq 1} \mathbb{G}_{M,q}$ .

*Proof.* The assertion is equivalent to say that we can choose for every  $M \in [0, 1]$  an  $\mathbf{f}^M \in \mathbb{A}_M$ , such that  $\mathcal{E}[\mathbf{f}^M]$  is uniformly bounded in  $M$ . This is easy to do. For example, let  $f$  be any nonnegative function in  $H^1 \cap L_V^2 \cap L^4$  such that  $\int f^2 = 1$ . Then for each  $M \in [0, 1]$ , let  $\mathbf{f}^M = ((\frac{1+M}{2})^{1/2} f, 0, (\frac{1-M}{2})^{1/2} f)$ . We have  $\mathbf{f}^M \in \mathbb{A}_M$  and

$$\mathcal{E}[\mathbf{f}^M] = \int \left\{ |\nabla f|^2 + V f^2 + \beta_n f^4 + \beta_s M^2 f^4 + q \right\},$$

which is bounded by the finite number  $\mathcal{E}[\mathbf{f}^1]$ .  $\square$

**Proposition 3.2.**  $E_g(\cdot, q)$  is strictly increasing on  $[0, 1]$ .

*Proof.* Let  $\mathbf{u} \in \mathbb{G}_{M,q}$ . We first consider  $0 < M \leq 1$ . For small  $\delta \geq 0$ , let  $\mathbf{u}(\delta)$  be the redistribution of  $\mathbf{u}$  defined by

$$\begin{cases} u_1(\delta)^2 = (1 - \delta)u_1^2 \\ u_0(\delta)^2 = u_0^2 + \delta u_1^2 + \delta u_{-1}^2 \\ u_{-1}(\delta)^2 = (1 - \delta)u_{-1}^2. \end{cases}$$

Then  $\mathbf{u}(\delta) \in \mathbb{A}_{(1-2\delta)M}$ . Since  $\mathbf{u}(\delta)$  is a redistribution of  $\mathbf{u}$ ,  $\mathcal{E}_{kin}[\mathbf{u}(\delta)] \leq \mathcal{E}_{kin}[\mathbf{u}]$ . One can also check by direct computation that

$$\mathcal{E}_{Zee}[\mathbf{u}] - \mathcal{E}_{Zee}[\mathbf{u}(\delta)] = q\delta \int (u_1^2 + u_{-1}^2) \geq 0,$$

and

$$\mathcal{E}_s[\mathbf{u}] - \mathcal{E}_s[\mathbf{u}(\delta)] = \beta_s \delta \int (u_1 - u_{-1})^2 [2u_0^2 + 4u_1 u_{-1} + \delta(u_1 - u_{-1})^2] \geq 0. \quad (3.3)$$

Moreover, if  $\delta > 0$ , strict inequality holds in (3.3). To see this, for  $0 < M < 1$ , note that  $u_1 u_{-1} > 0$  (Corollary 2.4) and the fact  $(u_1 - u_{-1})^2$  can not be identically zero. While for  $M = 1$ , only  $u_1 > 0$ , and the positivity of (3.3) is obvious. Thus we obtain

$$E_g((1 - 2\delta)M, q) \leq \mathcal{E}[\mathbf{u}(\delta)] < \mathcal{E}[\mathbf{u}] = E_g(M, q)$$

for each small  $\delta > 0$ , which shows  $E_g(\cdot, q)$  is strictly increasing on  $(0, 1]$ .

It remains to show that  $E_g(\cdot, q)$  is strictly increasing at 0. Let  $\{M_n\}$  be a sequence in  $(0, 1)$ ,  $M_n \rightarrow 0^+$ , and let  $\mathbf{u}^n \in \mathbb{G}_{M_n, q}$  for each  $n$ . By Lemma 3.1,  $\mathcal{E}[\mathbf{u}^n]$  is uniformly bounded, and hence Lemma 2.3 implies there is a subsequence  $\{\mathbf{u}^{n(k)}\}$  of  $\{\mathbf{u}^n\}$  such that  $\mathbf{u}^{n(k)} \rightharpoonup \mathbf{u}^\infty$  weakly in  $\mathbb{B}$  for some  $\mathbf{u}^\infty \in \mathbb{A}_0$ , and

$$E_g(0, q) \leq \mathcal{E}[\mathbf{u}^\infty] \leq \liminf_{k \rightarrow \infty} \mathcal{E}[\mathbf{u}^{n(k)}] = \liminf_{k \rightarrow \infty} E_g(M_{n(k)}, q) = \inf_{0 < M \leq 1} E_g(M, q).$$

Thus  $E_g(0, q) \leq E_g(M, q)$  for every  $M > 0$ . To see why strict inequality must hold, assume  $E_g(0, q) = E_g(M, q)$  for some  $M > 0$ , then since  $E_g(\cdot, q)$  is strictly increasing on  $(0, 1]$ , we have  $E_g(M/2, q) < E_g(0, q)$ , a contradiction.  $\square$

**Proposition 3.3.**  $E_g(\cdot, q)$  is continuous on  $[0, 1]$ .

*Proof.* The ideas of proving left continuity and right continuity are different. We first prove right continuity. Let  $\mathbf{u} \in \mathbb{G}_{M,q}$  for some  $0 \leq M < 1$ . For small  $\delta \geq 0$ , let  $\mathbf{u}(\delta)$  be the redistribution of  $\mathbf{u}$  defined by

$$\begin{cases} u_1(\delta)^2 = u_1^2 + \delta u_0^2 + \delta u_{-1}^2 \\ u_0(\delta)^2 = (1 - \delta)u_0^2 \\ u_{-1}(\delta)^2 = (1 - \delta)u_{-1}^2. \end{cases}$$

Let's use  $M_\delta$  to denote  $\mathcal{M}[\mathbf{u}(\delta)]$ . Then  $M_\delta = M + \delta \int (u_0^2 + 2u_{-1}^2)$ . Since  $0 \leq M < 1$ ,  $u_0$  and  $u_{-1}$  cannot both vanish, and hence  $M_\delta > M$  for  $\delta > 0$ , and  $M_\delta \rightarrow M^+$  as  $\delta \rightarrow 0^+$ . Now since  $E_g(\cdot, q)$  is strictly increasing, we have

$$0 < E_g(M_\delta, q) - E_g(M, q) \quad (3.4)$$

for  $\delta > 0$ . On the other hand, since  $\mathbf{u} \in \mathbb{G}_{M,q}$  while  $\mathbf{u}(\delta)$  need not be in  $\mathbb{G}_{M_\delta,q}$ , we have

$$\begin{aligned} E_g(M_\delta, q) - E_g(M, q) &\leq \mathcal{E}[\mathbf{u}(\delta)] - \mathcal{E}[\mathbf{u}] \\ &\leq (\mathcal{E}_s[\mathbf{u}(\delta)] - \mathcal{E}_s[\mathbf{u}]) + (\mathcal{E}_{Zee}[\mathbf{u}(\delta)] - \mathcal{E}_{Zee}[\mathbf{u}]) \end{aligned} \quad (3.5)$$

since  $\mathcal{E}_{kin}[\mathbf{u}(\delta)] \leq \mathcal{E}_{kin}[\mathbf{u}]$ . It's easy to check that by letting  $\delta \rightarrow 0^+$ , (3.5) implies

$$\limsup_{\delta \rightarrow 0^+} (E_g(M_\delta, q) - E_g(M, q)) \leq 0.$$

This together with (3.4) imply the right continuity of  $E_g(\cdot, q)$  on  $[0, 1]$ .

For left-continuity on  $(0, 1]$ , we prove by contradiction. Let  $M \in (0, 1]$ . Assume there is a sequence  $\{M_n\}$  in  $(0, 1)$  such that  $M_n \rightarrow M^-$  which  $E_g(M_n, q)$  doesn't converge to  $E_g(M, q)$ . By choosing a suitable subsequence, we can assume without loss of generality that  $E_g(M, q) - E_g(M_n, q) > \varepsilon$  for each  $n$ , for some  $\varepsilon > 0$ . Now let  $\{\mathbf{u}^n\}$  be such that  $\mathbf{u}^n \in \mathbb{G}_{M_n,q}$ , and let  $\{\mathbf{u}^{n(k)}\}$  and  $\mathbf{u}^\infty \in \mathbb{A}_M$  be as asserted in Lemma 2.3, we have

$$E_g(M, q) \leq \mathcal{E}[\mathbf{u}^\infty] \leq \liminf_{k \rightarrow \infty} \mathcal{E}[\mathbf{u}^{n(k)}] = \lim_{k \rightarrow \infty} E_g(M_{n(k)}, q) \leq E_g(M, q) - \varepsilon,$$

a contradiction. □

Proposition 3.3 implies the following important approximation result.

**Corollary 3.4.** For any  $M \in [0, 1]$ , we can find a sequence  $\{M_n\}$  in  $[0, 1]$  and a sequence  $\{\mathbf{u}^n\}$ ,  $\mathbf{u}^n \in \mathbb{G}_{M_n,q}$ , such that  $M_n \rightarrow M$ ,  $M_n \neq M$  for each  $n$ , and  $\mathbf{u}^n \rightarrow \mathbf{u}^\infty$  in  $\mathbb{B}$  for some  $\mathbf{u}^\infty \in \mathbb{G}_{M,q}$ .

*Proof.* Let  $\{M_n\}$  be a sequence in  $[0, 1]$  such that  $M_n \rightarrow M$  and  $M_n \neq M$  for each  $n$ . Let  $\{\mathbf{u}^n\}$  be such that  $\mathbf{u}^n \in \mathbb{G}_{M_n,q}$ . By definition  $\mathcal{N}[\mathbf{u}^n] = 1$  and  $\mathcal{M}[\mathbf{u}^n] \rightarrow M$ . Since  $\mathcal{E}[\mathbf{u}^n] = E_g(M_n, q)$ , by continuity of  $E_g(\cdot, q)$  we also have  $\mathcal{E}[\mathbf{u}^n] \rightarrow E_g(M, q)$ . Thus by Lemma 2.3,  $\{\mathbf{u}^n\}$  has a subsequence  $\{\mathbf{u}^{n(k)}\}$  such that  $\mathbf{u}^{n(k)} \rightarrow \mathbf{u}^\infty$  strongly in  $\mathbb{B}$  for some  $\mathbf{u}^\infty \in \mathbb{G}_{M,q}$ . The sequences  $\{M_{n(k)}\}$  and  $\{\mathbf{u}^{n(k)}\}$  satisfy the assertion of the corollary. □

### 3.1.2 $E_g$ as a function of $q$

Now we consider the function  $E_g(M, \cdot)$  for fixed  $M \in [0, 1]$ . For  $\mathbf{u} \in \mathbb{B}_+$ , let's temporarily write  $\mathcal{E}[\mathbf{u}, q]$  instead of  $\mathcal{E}[\mathbf{u}]$  to indicate its dependence on  $q$ . The proofs of monotonicity and continuity of  $E_g(M, \cdot)$  are much easier than those of  $E_g(\cdot, q)$  above, and the proof of continuity doesn't rely on the monotonicity. Indeed, if  $q_1 > q_2 \geq 0$ , let  $\mathbf{u} \in \mathbb{G}_{M, q_1}$ , we have

$$E_g(M, q_1) - E_g(M, q_2) \geq \mathcal{E}[\mathbf{u}, q_1] - \mathcal{E}[\mathbf{u}, q_2] = (q_1 - q_2) \int (u_1^2 + u_{-1}^2),$$

which implies  $E_g(M, \cdot)$  is an increasing function on  $[0, \infty)$ , and is strictly increasing if  $0 < M \leq 1$ .

On the other hand, for any  $q_1, q_2 \geq 0$  and  $\mathbf{u}^1 \in \mathbb{G}_{M, q_1}$ ,  $\mathbf{u}^2 \in \mathbb{G}_{M, q_2}$ , we have

$$(q_1 - q_2) \int ((u_1^1)^2 + (u_{-1}^1)^2) = \mathcal{E}[\mathbf{u}^1, q_1] - \mathcal{E}[\mathbf{u}^1, q_2] \leq E_g(M, q_1) - E_g(M, q_2), \quad (3.6)$$

and

$$E_g(M, q_1) - E_g(M, q_2) \leq \mathcal{E}[\mathbf{u}^2, q_1] - \mathcal{E}[\mathbf{u}^2, q_2] = (q_1 - q_2) \int ((u_1^2)^2 + (u_{-1}^2)^2). \quad (3.7)$$

From (3.6) and (3.7), and the fact  $\int ((u_1^k)^2 + (u_{-1}^k)^2) \leq 1$  for  $k = 1, 2$ , we find

$$|E_g(M, q_1) - E_g(M, q_2)| \leq |q_1 - q_2|,$$

and hence  $E_g(M, \cdot)$  is continuous. We summarize these results in the following proposition.

**Proposition 3.5.** *For fixed  $M \in [0, 1]$ ,  $E_g(M, \cdot)$  is an increasing and continuous function on  $[0, \infty)$ . Moreover, it's strictly increasing if  $0 < M \leq 1$ .*

*Remark 3.1.*  $E_g(0, \cdot)$  is not strictly increasing. Indeed, by Proposition (3.7) below, for  $q > 0$ ,  $\mathbf{u} \in \mathbb{G}_{0, q}$  satisfies  $u_1 = u_{-1} = 0$ . Such one-component ground state is unique and independent of  $q$  (see Remark 2.2). Thus  $E_g(0, \cdot)$  is a constant function on  $(0, \infty)$ , and hence on  $[0, \infty)$  by continuity.

With the continuity of  $E_g(M, \cdot)$  we can prove the analogue of Corollary 3.4 for fixed  $M$  and varied  $q$ . The proof is the same as that of Corollary 3.4 by changing the roles of  $M$  and  $q$ , and is omitted.

**Corollary 3.6.** *Fix  $M \in [0, 1]$ . For any  $q \geq 0$ , we can find a sequence  $\{q_n\}$  in  $[0, \infty)$  and a sequence  $\{\mathbf{u}^n\}$ ,  $\mathbf{u}^n \in \mathbb{G}_{M, q_n}$ , such that  $q_n \rightarrow q$ ,  $q_n \neq q$  for each  $n$ , and  $\mathbf{u}^n \rightarrow \mathbf{u}^\infty$  in  $\mathbb{B}$  for some  $\mathbf{u}^\infty \in \mathbb{G}_{M, q}$ .*

### 3.2 $u_{-1}$ is no larger than $u_1$

We show in this subsection that  $u_{-1} \leq u_1$  for any  $\mathbf{u} \in \mathbb{G}_{M,q}$ . With the aid of this fact we will prove  $\mathbf{u}(x)$  decays exponentially as  $|x| \rightarrow \infty$ .

**Proposition 3.7.** *Let  $\mathbf{u} \in \mathbb{G}_{0,q}$ . If  $q > 0$ , then  $u_1 = u_{-1} = 0$ .*

*Proof.* Let  $\mathbf{v}$  be the element in  $\mathbb{A}_0$  defined by

$$\begin{cases} v_1^2 = v_{-1}^2 = (u_1^2 + u_{-1}^2)/2 \\ v_0^2 = u_0^2. \end{cases}$$

Then  $\mathcal{E}[\mathbf{u}] - \mathcal{E}[\mathbf{v}] = (\mathcal{E}_{kin}[\mathbf{u}] - \mathcal{E}_{kin}[\mathbf{v}]) + \mathcal{E}_s[\mathbf{u}]$ . Since  $\mathbf{v}$  is a redistribution of  $\mathbf{u}$ ,  $\mathcal{E}_{kin}[\mathbf{u}] - \mathcal{E}_{kin}[\mathbf{v}] \geq 0$ . Also,  $\mathcal{E}_s[\mathbf{u}] \geq 0$ , and hence  $\mathcal{E}[\mathbf{u}] - \mathcal{E}[\mathbf{v}] \geq 0$ . But  $\mathbf{u} \in \mathbb{G}_{0,q}$ , so we must have  $\mathcal{E}[\mathbf{u}] - \mathcal{E}[\mathbf{v}] = 0$ . Thus actually  $\mathcal{E}_{kin}[\mathbf{u}] - \mathcal{E}_{kin}[\mathbf{v}] = \mathcal{E}_s[\mathbf{u}] = 0$ , which implies  $u_1 = u_{-1}$ . To see why they must vanish, note that

$$\begin{aligned} \mathcal{E}[\mathbf{u}] &= \int \left\{ \sum_j |\nabla u_j|^2 + V(x)|\mathbf{u}|^2 + \beta_n |\mathbf{u}|^4 + q(u_1^2 + u_{-1}^2) \right\} \\ &\geq \int \{ |\nabla |\mathbf{u}||^2 + V(x)|\mathbf{u}|^2 + \beta_n |\mathbf{u}|^4 \} = \mathcal{E}[(0, |\mathbf{u}|, 0)]. \end{aligned} \quad (3.8)$$

Again since  $\mathbf{u} \in \mathbb{G}_{0,q}$  and  $(0, |\mathbf{u}|, 0) \in \mathbb{A}_0$ , we must have  $\mathcal{E}[\mathbf{u}] = \mathcal{E}[(0, |\mathbf{u}|, 0)]$ . Thus equality holds in (3.8). This can happen only if  $\mathbf{u} = (0, |\mathbf{u}|, 0)$  since  $\sum_j |\nabla u_j|^2 \geq |\nabla |\mathbf{u}||^2$  and  $q > 0$ .  $\square$

*Remark 3.2.* For  $M = q = 0$ , we also have  $u_1 = u_{-1}$  but ground states are not unique. The case  $u_1 = u_{-1} = 0$  corresponds to only one possibility. See [20], Theorem 4.2.

**Proposition 3.8.** *For every  $0 \leq M \leq 1$  and  $q \geq 0$ ,  $\mathbf{u} \in \mathbb{G}_{M,q}$  satisfies  $u_{-1} \leq u_1$ .*

*Proof.* Let  $\mathbf{v}$  be defined by  $v_1 = \max(u_1, u_{-1})$ ,  $v_{-1} = \min(u_1, u_{-1})$ , and  $v_0 = u_0$ . Then we have  $\mathcal{E}[\mathbf{v}] = \mathcal{E}[\mathbf{u}]$ . To check this equality, for the kinetic part  $\mathcal{E}_{kin}$  one can use the formula

$$v_j = \frac{1}{2}(u_j + u_{-j} + j|u_j - u_{-j}|)$$

for  $j = 1, -1$ , and the fact  $|\nabla |f||^2 = |\nabla f|^2$  a.e. for any  $f \in H^1$ . The equalities of the other parts are obvious. Thus  $E_g(\mathcal{M}[\mathbf{v}], q) \leq E_g(M, q)$ , and we have

$$\mathcal{M}[\mathbf{v}] \leq M \quad (3.9)$$

since  $E_g(\cdot, q)$  is strictly increasing. On the other hand, it's also obvious by definition that

$$v_1^2 - v_{-1}^2 \geq u_1^2 - u_{-1}^2. \quad (3.10)$$

(3.9) and (3.10) imply  $v_1^2 - v_{-1}^2 = u_1^2 - u_{-1}^2$ , that is  $v_1^2 - u_1^2 = v_{-1}^2 - u_{-1}^2$ , of which the left-hand side is nonnegative while the right-hand side is nonpositive by definition of  $\mathbf{v}$ . Thus we really have  $v_1 = u_1$  and  $v_{-1} = u_{-1}$ , which means  $u_{-1} \leq u_1$ .  $\square$

**Corollary 3.9.** *Let  $\mathbf{u} \in \mathbb{G}_{M,q}$ . If  $0 < M < 1$ , the Lagrange multiplier  $\lambda$  in the GP system (2.2) is positive.*

*Proof.* (2.2a) multiplied by  $u_{-1}$  minus (2.2c) multiplied by  $u_1$  gives

$$2\lambda u_1 u_{-1} = \nabla \cdot (-u_{-1} \nabla u_1 + u_1 \nabla u_{-1}) + 2\beta_s (u_1^2 - u_{-1}^2)(u_0^2 + 2u_1 u_{-1}). \quad (3.11)$$

Thus

$$\lambda \int u_1 u_{-1} = \beta_s \int (u_1^2 - u_{-1}^2)(u_0^2 + 2u_1 u_{-1}). \quad (3.12)$$

To justify (3.12) carefully, we can test (3.11) by  $\varphi_R(|x|)$ , where  $\varphi_R : [0, \infty) \rightarrow [0, 1]$  is defined by

$$\varphi_R(r) = \begin{cases} 1, & r \leq R \\ R+1-r, & R < r \leq R+1 \\ 0, & R+1 < r, \end{cases}$$

and then let  $R$  go to infinity.

Now  $u_1 u_{-1} > 0$  by Corollary 2.4, and hence  $\int u_1 u_{-1} > 0$ . On the other hand, by Proposition 3.8 we have  $u_1^2 - u_{-1}^2 \geq 0$ , which cannot be identically zero since  $M > 0$ . Thus we also have  $\int (u_1^2 - u_{-1}^2)(u_0^2 + 2u_1 u_{-1}) > 0$ , and (3.12) implies  $\lambda > 0$ .  $\square$

It's interesting that with this corollary of Proposition 3.8, we can further sharpen the assertion of Proposition 3.8.

**Proposition 3.10.** *For  $0 < M \leq 1$  and  $q \geq 0$ ,  $\mathbf{u} \in \mathbb{G}_{M,q}$  satisfies  $u_{-1} < u_1$ .*

*Proof.* If  $M = 1$ , we have  $u_1 > 0 = u_{-1}$ . For  $0 < M < 1$ , let  $w = u_1 - u_{-1}$ . Then (2.2a) minus (2.2c) gives

$$\Delta w + Qw = -\lambda(u_1 + u_{-1}) - \mu w, \quad (3.13)$$

where  $Q = -V - 2\beta_n |\mathbf{u}|^2 - 2\beta_s [2u_0^2 + (u_1 + u_{-1})^2] - q \leq 0$ . Since  $\lambda > 0$  and  $w \geq 0$ , by subtracting  $|\mu|w$  from both sides of (3.13), we obtain  $\Delta w + \tilde{Q}w \leq 0$ , where  $\tilde{Q} = Q - |\mu| \leq 0$ . By the strong minimum principle either  $w > 0$  everywhere or  $w \equiv 0$ . But  $w \equiv 0$  means  $u_1 = u_{-1}$ , contradicting to the assumption  $M > 0$ . Thus  $w > 0$ , which is what we want.  $\square$

*Remark 3.3.* Recall that we denote the unique element in  $\mathbb{G}_{M,q}^{two}$  by  $\mathbf{z}^M$ , which is independent of  $q$ . Assume  $0 < M \leq 1$ , then we also have  $z_{-1}^M < z_1^M$ . This is because  $\mathbf{z}^M$  is just the element in  $\mathbb{G}_{M,0}$  from [20].

With the aid of Proposition 3.8, we now prove the exponential decaying of ground states. The approach by using Yukawa potential is exactly taken from Lemma A.5 of [18].

**Proposition 3.11.** *Let  $\mathbf{u} \in \mathbb{G}_{M,q}$  for arbitrary  $0 \leq M \leq 1$  and  $q \geq 0$ . For any  $t > 0$ , there exists  $M_j(t)$  ( $j = 1, 0, -1$ ) such that  $u_j(x) \leq M_j(t)e^{-t|x|}$ .*

*Proof.* (2.2b) can be arranged as

$$(-\Delta + t^2)u_0 = Q_0u_0,$$

where

$$Q_0 = t^2 + \mu - V - 2\beta_n|\mathbf{u}|^2 - 2\beta_s(u_1 - u_{-1})^2. \quad (3.14)$$

Thus

$$u_0(x) = \int Y_t(x-y)Q_0(y)u_0(y)dy,$$

where  $Y_t(x) = e^{-t|x|}/(4\pi|x|)$  is the fundamental solution of the operator  $-\Delta + t^2$  (also referred to as the Yukawa potential. See [17], 6.23). By the assumption (A1),  $Q_0 < 0$  outside a bounded set, say  $B(R_0)$ , the open ball centered at the origin with radius  $R_0$ . Thus we obtain

$$u_0(x) \leq \int_{|y| < R_0} Y_t(x-y)Q_0(y)u_0(y)dy = e^{-t|x|} \int_{|y| < R_0} \frac{e^{t(|x|-|x-y|)}}{4\pi|x-y|} Q_0(y)u_0(y)dy.$$

Thus  $u_0(x) \leq M_0(t)e^{-t|x|}$ , where

$$M_0(t) = \sup_{x \in \mathbb{R}^3} \int_{|y| < R_0} \frac{e^{t(|x|-|x-y|)}}{4\pi|x-y|} Q_0(y)u_0(y)dy. \quad (3.15)$$

For  $u_j$ ,  $j = 1, -1$ , we similarly have

$$(-\Delta + t^2)u_j = Q_ju_j - 2\beta_su_0^2(u_j - u_{-j})$$

from (2.2a) and (2.2c), where

$$Q_j = t^2 + \mu + j\lambda - V - 2\beta_n|\mathbf{u}|^2 - 2\beta_s(u_j^2 - u_{-j}^2) - q.$$

Now since  $u_{-1} \leq u_1$ ,  $Q_1$  is also negative outside  $B(R_1)$  for some radius  $R_1$ , and

$$\begin{aligned} u_1(x) &= \int Y_t(x-y)[Q_1(y)u_1(y) - 2\beta_su_0(y)^2(u_1(y) - u_{-1}(y))]dy \\ &\leq \int Y_t(x-y)Q_1(y)u_1(y)dy \\ &\leq \int_{|y| < R_1} Y_t(x-y)Q_1(y)u_1(y)dy. \end{aligned}$$

As above we conclude that  $u_1(x) \leq M_1(t)e^{-t|x|}$ , where  $M_1(t)$  is given by (3.15) with all the indices 0 replaced by 1. In contrast, the fact  $u_{-1} \leq u_1$  makes it difficult to apply the same argument to  $u_{-1}$ . Nevertheless, also since  $u_{-1} \leq u_1$ , at least we can choose  $M_{-1}(t) = M_1(t)$ .  $\square$

Later we will consider ground states corresponding to different values of  $M$  and  $q$ , and hence different Lagrange multipliers. The following observation will be useful.

**Lemma 3.12.** *For  $\mu$  and  $\lambda$  in bounded sets,  $M_j(t)$  can be chosen to be independent of  $\mu$  and  $\lambda$ .*

*Proof.* Take  $M_0(t)$  for example. Assume  $\mu < C$  for some constant  $C > 0$ . From (3.14),  $Q_0 \leq t^2 + \mu - V < t^2 + C - V$ , and hence  $R_0$  can be chosen to be independent of  $\mu$  (and  $\lambda$ ). Then by Hölder inequality and the fact  $\int u_0^2 \leq \int |\mathbf{u}|^2 = 1$ , (3.15) gives

$$\begin{aligned} M_0(t) &\leq \sup_{x \in \mathbb{R}^3} \left( \int_{|y| < R_0} \frac{e^{2t(|x|-|x-y|)}}{16\pi^2|x-y|^2} Q_0(y)^2 dy \right)^{1/2} \\ &\leq \sup_{x \in \mathbb{R}^3} \left( \int_{|y| < R_0} \frac{e^{2t(|x|-|x-y|)}}{16\pi^2|x-y|^2} (t^2 + C - V(y))^2 dy \right)^{1/2}. \end{aligned}$$

$M_1(t)$  can be estimated similarly, and the assertion for  $M_{-1}(t)$  follows.  $\square$

## 4 Redistributinal Perturbation in a Fixed Admissible Class

Let  $\mathbf{u} \in \mathbb{G}_{M,q}$ . We have seen it's sometimes useful to construct a ‘‘redistributinal perturbation’’  $\mathbf{u}(\delta)$  of  $\mathbf{u}$ . In previous examples (namely Proposition 3.2 and Proposition 3.3), the  $\mathbf{u}(\delta)$  are so constructed to be in different  $\mathbb{A}_{M'}$ , in order to compare ground states with different magnetizations. In this section we investigate the idea, possibly more natural, of perturbing  $\mathbf{u}$  in the same class. Then, since  $\mathcal{E}[\mathbf{u}] \leq \mathcal{E}[\mathbf{u}(\delta)]$  for each  $\delta \geq 0$ , we have

$$\left. \frac{d}{d\delta} \mathcal{E}[\mathbf{u}(\delta)] \right|_{\delta=0^+} = \left. \frac{d}{d\delta} \mathcal{E}_{kin}[\mathbf{u}(\delta)] \right|_{\delta=0^+} + \left. \frac{d}{d\delta} \mathcal{E}_s[\mathbf{u}(\delta)] \right|_{\delta=0^+} + \left. \frac{d}{d\delta} \mathcal{E}_{Zee}[\mathbf{u}(\delta)] \right|_{\delta=0^+} \geq 0, \quad (4.1)$$

as long as the derivatives exist. Here  $\left. \frac{d}{d\delta}(\cdot) \right|_{\delta=0^+}$  denotes right differentiation at  $\delta = 0$ . It turns out that the existence of such derivatives need some verification. In the following we give two examples, Proposition 4.1 and Proposition 4.2, which will be useful in the next section. We first introduce some notations.

- For  $\delta > 0$ , we will use  $D(\mathbf{u}(\delta))$  to denote the difference quotient  $(H(\mathbf{u}(\delta)) - H(\mathbf{u}))/\delta$ . Thus  $\left. \frac{d}{d\delta} \mathcal{E}[\mathbf{u}(\delta)] \right|_{\delta=0^+} = \lim_{\delta \rightarrow 0^+} \int D(\mathbf{u}(\delta))$ , which equals  $\int \left. \frac{\partial}{\partial \delta} H(\mathbf{u}(\delta)) \right|_{\delta=0^+}$  if we can differentiate it under the integral sign. Similarly,  $D_{kin}(\mathbf{u}(\delta))$ ,  $D_s(\mathbf{u}(\delta))$  and  $D_{Zee}(\mathbf{u}(\delta))$  are understood to be the difference quotients of the indicated parts of  $H(\mathbf{u}(\delta))$ .
- For  $\mathbf{u} \in \mathbb{G}_{M,q}$ , we write  $S(u_i, u_j) = |u_i \nabla u_j - u_j \nabla u_i|^2$ . When computing  $D_{kin}(\mathbf{u}(\delta))$ , we will use the following formula:

$$\sum_j a_j |\nabla u_j|^2 - \left| \nabla \left( \sum_j a_j u_j^2 \right)^{1/2} \right|^2 = \frac{\sum_{k < \ell} a_k a_\ell S(u_k, u_\ell)}{\sum_j a_j u_j^2}$$

if  $\sum_j a_j u_j^2 > 0$ , where  $a_j$  ( $j = 1, 0, -1$ ) are nonnegative constants.

**Proposition 4.1.** For  $0 < M < 1$  and  $q \geq 0$ , if  $\mathbf{z}^M$  is a ground state, i.e.  $\mathbf{z}^M \in \mathbb{G}_{M,q}$ , then

$$4\beta_s \int z_1^M z_{-1}^M (z_1^M - z_{-1}^M)(\tau z_{-1}^M - z_1^M) \geq q(1+M) + \int \frac{\tau S(z_1^M, z_{-1}^M)}{(z_1^M)^2 + \tau(z_{-1}^M)^2}, \quad (4.2)$$

where  $\tau = (\int z_1^2)/(\int z_{-1}^2) = (1+M)/(1-M)$ .

*Proof.* In this proof we omit the superscript  $M$  of  $\mathbf{z}^M$  for simplicity. Consider the redistribution  $\mathbf{u}(\delta)$  of  $\mathbf{z}$  defined by

$$\begin{cases} u_1(\delta)^2 = (1-\delta)z_1^2 \\ u_0(\delta)^2 = \delta z_1^2 + \tau \delta z_{-1}^2 \\ u_{-1}(\delta)^2 = (1-\tau\delta)z_{-1}^2. \end{cases}$$

It's easy to check  $\mathbf{u}(\delta) \in \mathbb{A}_M$  for each small  $\delta > 0$ . We compute  $\frac{d}{d\delta}\mathcal{E}[\mathbf{u}(\delta)]\Big|_{\delta=0^+}$  as follows: First,

$$D_{kin}(\mathbf{u}(\delta)) = \frac{1}{\delta} \left\{ |\nabla u_0(\delta)|^2 - (\delta|\nabla z_1|^2 + \tau\delta|\nabla z_{-1}|^2) \right\} = -\frac{\tau S(z_1, z_{-1})}{z_1^2 + \tau z_{-1}^2},$$

which is independent of  $\delta$ , and hence

$$\frac{d}{d\delta}\mathcal{E}_{kin}[\mathbf{u}(\delta)]\Big|_{\delta=0^+} = -\int \frac{\tau S(z_1, z_{-1})}{z_1^2 + \tau z_{-1}^2}.$$

Second, for  $\delta \geq 0$  in a fixed small neighborhood of 0, it's easy to check

$$\left| \frac{\partial}{\partial \delta} H_s(\mathbf{u}(\delta)) \right| \leq C|\mathbf{z}|^4$$

for some  $C$  independent of  $\delta$ . Thus it's valid to differentiate  $\mathcal{E}_s[\mathbf{u}(\delta)]$  under the integral sign, which gives

$$\begin{aligned} \frac{d}{d\delta}\mathcal{E}_s[\mathbf{u}(\delta)]\Big|_{\delta=0^+} &= 2\beta_s \int \left\{ (z_1^2 + \tau z_{-1}^2)(z_1 - z_{-1})^2 + (z_1^2 - z_{-1}^2)(-z_1^2 + \tau z_{-1}^2) \right\} \\ &= 4\beta_s \int z_1 z_{-1} (z_1 - z_{-1})(\tau z_{-1} - z_1). \end{aligned}$$

Finally,  $\mathcal{E}_{Zee}[\mathbf{u}(\delta)] = q[(1-\delta) \int z_1^2 + (1-\tau\delta) \int z_{-1}^2]$ , and we have

$$\frac{d}{d\delta}\mathcal{E}_{Zee}[\mathbf{u}(\delta)]\Big|_{\delta=0^+} = q \left( -\int z_1^2 - \tau \int z_{-1}^2 \right) = -q(1+M).$$

The assertion now follows  $\frac{d}{d\delta}\mathcal{E}[\mathbf{u}(\delta)]\Big|_{\delta=0^+} \geq 0$ .  $\square$

**Proposition 4.2.** For  $0 < M < 1$  and  $q \geq 0$ , any  $\mathbf{u} \in \mathbb{G}_{M,q}$  satisfies

$$q \int u_0^2 \geq \beta_s \int u_0^2 (u_1 - u_{-1})^2 \left( 2 + \frac{u_0^2}{u_1 u_{-1}} \right) + \frac{1}{2} \int \sum_{j=1,-1} \frac{S(u_j, u_0)}{u_j^2}. \quad (4.3)$$

*Proof.* Let  $\mathbf{u}(\delta)$  be defined by

$$\begin{cases} u_1(\delta)^2 = u_1^2 + \delta u_0^2 \\ u_0(\delta)^2 = (1 - 2\delta)u_0^2 \\ u_{-1}(\delta)^2 = u_{-1}^2 + \delta u_0^2. \end{cases}$$

It's easy to see  $\mathbf{u}(\delta) \in \mathbb{A}_M$  for each small  $\delta > 0$ . Now

$$\left. \frac{d}{d\delta} \mathcal{E}_{Zee}[\mathbf{u}(\delta)] \right|_{\delta=0^+} = \lim_{\delta \rightarrow 0^+} \int D_{Zee}(\mathbf{u}(\delta)) = 2q \int u_0^2.$$

On the other hand, it's not obvious whether we can differentiate  $\mathcal{E}_{kin}[\mathbf{u}(\delta)]$  and  $\mathcal{E}_s[\mathbf{u}(\delta)]$  under the integral signs. We could avoid this problem as follows. Since  $\int D(\mathbf{u}(\delta)) \geq 0$ ,

$$\int D_{Zee}(\mathbf{u}(\delta)) \geq - \int D_s(\mathbf{u}(\delta)) - \int D_{kin}(\mathbf{u}(\delta)). \quad (4.4)$$

Now  $D_{kin}(\mathbf{u}(\delta)) \leq 0$  since  $\mathbf{u}(\delta)$  is a redistribution of  $\mathbf{u}$ . Also, it's easy to check that  $\frac{\partial}{\partial \delta} H_s(\mathbf{u}(\delta)) \leq 0$  for small  $\delta > 0$ , and hence  $D_s(\mathbf{u}(\delta)) \leq 0$  for small  $\delta > 0$ . Thus, after taking liminf as  $\delta \rightarrow 0^+$ , we can apply Fatou's lemma to the right-hand side of (4.4), and we obtain

$$2q \int u_0^2 \geq \int - \left. \frac{\partial}{\partial \delta} H_s(\mathbf{u}(\delta)) \right|_{\delta=0^+} + \int - \left. \frac{\partial}{\partial \delta} H_{kin}(\mathbf{u}(\delta)) \right|_{\delta=0^+}. \quad (4.5)$$

It's easy to check that, divided by 2, (4.5) gives (4.3).  $\square$

*Remark 4.1.* Now that the terms of the right-hand side of (4.3) are finite,  $u_0^4(u_1 - u_{-1})^2/(u_1 u_{-1})$  and  $S(u_j, u_0)/u_j^2$  ( $j = 1, -1$ ) are integrable. We can use them to find suitable bounds of  $\left| \frac{\partial}{\partial \delta} H_s(\mathbf{u}(\delta)) \right|$  and  $\left| \frac{\partial}{\partial \delta} H_{kin}(\mathbf{u}(\delta)) \right|$  independent of small  $\delta > 0$ , and conclude that  $\mathcal{E}_s[\mathbf{u}(\delta)]$  and  $\mathcal{E}_{kin}[\mathbf{u}(\delta)]$  can really be differentiated under the integral sign. One might suspect such operations of taking differentiation should be valid for all similar constructions of  $\mathbf{u}(\delta)$ . This is probably true. However, there are cases of which the validity is not easy to see. See Section 6.3 for further discussion.

There is another point of view on what we did above, which leads us to find (4.3) is really an equality but not merely an inequality. We discuss it in the following. At any rate, a redistributional perturbation  $\mathbf{u}(\delta)$  is a kind of perturbation, and it's natural to suspect that the results above could also be obtained from the GP system (2.2), which consists of information from general perturbations. Indeed, using chain rule formally we

have  $\frac{d}{d\delta}\mathcal{E}[\mathbf{u}(\delta)]\Big|_{\delta=0^+} = \mathcal{E}'[\mathbf{u}](\mathbf{u}'(0^+))$ , and one would expect (4.1) might be a consequence of testing (2.2) by  $\mathbf{u}'(0^+)$ . This inference is not totally rigorous. Most importantly, we are not sure whether  $\mathbf{u}'(0^+)$  is good enough (for example in  $\mathbb{B}$ ) so that  $\mathcal{E}'[\mathbf{u}](\mathbf{u}'(0^+))$  makes sense. It turns out that we can really prove equality holds in (4.3) by using the GP system, while in our argument the inequality itself plays a critical role. We demonstrate this claim in the rest of this section. For this we first give a lemma.

**Lemma 4.3.** *Let  $f : \mathbb{R}^3 \rightarrow \mathbb{R}$  and  $\mathbf{g} = (g_1, g_2, g_3) : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  be continuous. Assume  $|f(x)| = O(|x|^{-1})$  as  $|x| \rightarrow \infty$ , and  $|\mathbf{g}| \in L^2$ . Then if  $\nabla \cdot (f\mathbf{g})$  (as a distribution) is in  $L^1$ , we have  $\int \nabla \cdot (f\mathbf{g}) = 0$ .*

*Proof.* Write  $\nabla \cdot (f\mathbf{g}) = h$ . Then

$$\int h = \lim_{r \rightarrow \infty} \int_{\partial B(r)} f\mathbf{g} \cdot \mathbf{n}, \quad (4.6)$$

where  $\mathbf{n}$  is the unit outer normal on  $\partial B(r)$ . Let's denote  $|\int_{\partial B(r)} f\mathbf{g} \cdot \mathbf{n}|$  by  $I(r)$ , and our goal is to prove  $\lim_{r \rightarrow \infty} I(r) = 0$ . By assumption, for  $|x|$  large,  $|f(x)| \leq C|x|^{-1}$  for some constant  $C > 0$ , and hence for  $r$  large enough we have

$$I(r) \leq C|r|^{-1} \int_{\partial B(r)} |\mathbf{g}| \leq C|r|^{-1} \left( \int_{\partial B(r)} |\mathbf{g}|^2 \right)^{1/2} |\partial B(r)|^{1/2} = \tilde{C} \left( \int_{\partial B(r)} |\mathbf{g}|^2 \right)^{1/2}$$

by Hölder's inequality, where  $|\partial B(r)|$  denotes the area of  $\partial B(r)$  and  $\tilde{C} = C|\partial B(1)|^{1/2}$ . As a consequence, we have

$$\int |\mathbf{g}|^2 = \int_0^\infty \left( \int_{\partial B(r)} |\mathbf{g}|^2 \right) dr \geq \tilde{C}^{-2} \int_0^\infty I(r)^2 dr, \quad (4.7)$$

which is finite since  $|\mathbf{g}| \in L^2$ . Note that by (4.6),  $\lim_{r \rightarrow \infty} I(r)$  does exist, and it must be zero by (4.7).  $\square$

It's also convenient to give the following computational result first. The proof is straightforward and omitted.

**Lemma 4.4.** *Assume  $f, g \in C^1$  and  $f, g > 0$ , then*

$$g^2 \left( \frac{\Delta f}{f} - \frac{\Delta g}{g} \right) = -\nabla \cdot \left( fg \nabla \left( \frac{g}{f} \right) \right) + \left| f \nabla \left( \frac{g}{f} \right) \right|^2,$$

*which is regarded as an identity of distributions.*

We can now prove the promised result.

**Theorem 4.5.** *The inequality (4.3) is an equality.*

*Proof.* Let  $\mathbf{u}(\delta)$  be as in the proof of Proposition 4.2. Then

$$\mathbf{u}'(0^+) = \left( u_0^2/(2u_1), -u_0, u_0^2/(2u_{-1}) \right).$$

From the discussion before Lemma 4.3, this indicates we do the following: Multiplying (2.2a) by  $u_0^2/(2u_1)$ , multiplying (2.2b) by  $-u_0$ , and multiplying (2.2c) by  $u_0^2/(2u_{-1})$ . Summing these three equations, and after some rearrangement, we obtain

$$qu_0^2 = \beta_s u_0^2 (u_1 - u_{-1})^2 \left( 2 + \frac{u_0^2}{u_1 u_{-1}} \right) + \frac{1}{2} \sum_{j=1,-1} u_0^2 \left( \frac{\Delta u_j}{u_j} - \frac{\Delta u_0}{u_0} \right). \quad (4.8)$$

Now by Lemma 4.4, for  $j = 1, -1$  we have

$$u_0^2 \left( \frac{\Delta u_j}{u_j} - \frac{\Delta u_0}{u_0} \right) = -\nabla \cdot \left( u_0 u_j \nabla \left( \frac{u_0}{u_j} \right) \right) + \left| u_j \nabla \left( \frac{u_0}{u_j} \right) \right|^2. \quad (4.9)$$

Note that  $|u_j \nabla (u_0/u_j)|^2$  is just  $S(u_j, u_0)/u_j^2$ , and hence it remains to show

$$\int \nabla \cdot \left( u_0 u_j \nabla \left( \frac{u_0}{u_j} \right) \right) = 0.$$

For this we check the conditions in Lemma 4.3 with  $f = u_0$  and  $\mathbf{g} = u_j \nabla (u_0/u_j)$ . First, from Proposition 3.11,  $u_0(x) = O(|x|^{-1})$ . Then, from (4.3),  $S(u_j, u_0)/u_j^2$  is integrable, which means  $|u_j \nabla (u_0/u_j)| \in L^2$ . Finally, from (4.8), (4.9) and (4.3),  $\nabla \cdot (u_0 u_j \nabla (u_0/u_j))$  is really in  $L^1$ , and the proof is completed.  $\square$

*Remark 4.2.* To eliminate the unwanted term  $\nabla \cdot (u_0 u_j \nabla (u_0/u_j))$ , in the proof above we use the inequality (4.3) at two places: to guarantee that  $|u_j \nabla (u_0/u_j)| \in L^2$ , and to guarantee  $\nabla \cdot (u_0 u_j \nabla (u_0/u_j)) \in L^1$ . It looks somewhat pedantic, but seems unavoidable. For example, from (4.8) alone, we do not even know if  $u_0^2 (u_1 - u_{-1})^2 (2 + u_0^2/(u_1 u_{-1}))$  is in  $L^1$ . We remark that similar problems happen to other constructions of  $\mathbf{u}(\delta)$  which lead to equalities. Thus in our context the inequalities obtained from redistribution are not consequences of the GP system. This declaration however may be overthrown if we can prove some comparison results of the asymptotic behaviors of the three components. See Section 6.3 for discussion.

*Remark 4.3.* We'd like to do the same thing for (4.2). However, note that since  $\mathbf{z}^M$  is independent of  $q$ , it's impossible that (4.2) be an equality for varied  $q$ . Indeed, following the idea of proving Theorem 4.5, we get a trouble at the very beginning: by letting  $\mathbf{u}(\delta)$  be defined as in the proof of Proposition 4.1, we have  $\mathbf{u}'(0^+) = (-z_1^M/2, +\infty, -\tau z_{-1}^M/2)$ , which suggests we multiply (2.2b) for  $\mathbf{z}^M$  (which is the trivial equation  $0 = 0$ ) by infinity. This problem can be avoided if there is a sequence  $\mathbf{u}^n$  of ground states (corresponding to different values of  $M$  or  $q$  or both) such that  $u_n > 0$ , and  $u_0^n$  tends to zero. The details will be given in Section 5.2.

## 5 Bifurcation Between 2C and 3C Ground States

In this section we study the bifurcation between the 2C regime and the 3C regime of ground states for  $(M, q) \in (0, 1) \times (0, \infty)$ . (We recommend the reader Figure 5 of [19] for a clear illustration.) In [20], we proved that for  $0 < M < 1$ ,  $\mathbf{u} \in \mathbb{G}_{M,0}$  implies  $u_0 = 0$ , i.e.  $\mathbf{u} = \mathbf{z}^M$ . According to numerical results, if  $q$  is not too large, ground state remains 2C, while for  $q$  greater than some critical value  $u_0$  emerges. We prove this observation in Section 5.1. Some characterizations of the bifurcation points are given in Section 5.2.

### 5.1 Existence of bifurcation point

The observation we are going to prove is summarized as the following theorem.

**Theorem 5.1.** *For  $0 < M < 1$ , there is a  $q_c(M) > 0$  such that for  $q > q_c(M)$  (resp.  $q < q_c(M)$ ),  $\mathbf{u} \in \mathbb{G}_{M,q}$  implies  $u_0 > 0$  (resp.  $\mathbf{u} = \mathbf{z}^M$ ).*

The proof is separated into several parts. Roughly speaking, our idea is using (4.2) to disprove  $u_0 \equiv 0$ , and using (4.3) to disprove  $u_0 > 0$ . In the following we fix an  $M \in (0, 1)$ .

**Claim 1** For  $q$  large enough, if  $\mathbf{u} \in \mathbb{G}_{M,q}$ , we have  $u_0 > 0$ .

*Proof.* Assume  $\mathbf{z}^M \in \mathbb{G}_{M,q}$ , then  $\mathbf{z}^M$  satisfies (4.2). Since  $\mathbf{z}^M$  is independent of  $q$ , it indeed gives an upper bound for  $q$ , and hence the assertion.  $\square$

**Claim 2** Assume for some  $q$  there exists  $\mathbf{u} \in \mathbb{G}_{M,q}$  with  $u_0 > 0$ , then for every  $q' > q$ ,  $\mathbf{v} \in \mathbb{G}_{M,q'}$  satisfies  $v_0 > 0$ .

*Proof.* Let's use  $\mathcal{E}[\cdot, q]$  instead of  $\mathcal{E}[\cdot]$  to specify the value of  $q$ . Since  $\mathbf{u} \in \mathbb{G}_{M,q}$ ,  $\mathcal{E}[\mathbf{u}, q] \leq \mathcal{E}[\mathbf{z}^M, q]$ . Thus, by the assumption  $u_0 > 0$ , we have  $\mathcal{E}[\mathbf{u}, q'] < \mathcal{E}[\mathbf{z}^M, q']$  for any  $q' > q$ . Hence  $\mathbf{z}^M \notin \mathbb{G}_{M,q'}$  for  $q' > q$ , which is what we want to show.  $\square$

Now define

$$q_c(M) = \inf \left\{ q \mid \text{for any } q' > q, \mathbf{v} \in \mathbb{G}_{M,q'} \text{ have } v_0 > 0 \right\}.$$

From Claim 1,  $q_c(M) < \infty$ . By definition for any  $q > q_c(M)$  and  $\mathbf{v} \in \mathbb{G}_{M,q}$ , we have  $v_0 > 0$ . Moreover, since  $q_c(M)$  is the infimum of all numbers satisfying this property, Claim 2 implies  $q_c(M)$  also satisfies the following property: For any  $0 \leq q < q_c(M)$  and  $\mathbf{v} \in \mathbb{G}_{M,q}$ ,  $v_0 = 0$ . To complete the proof of Theorem 5.1, it remains to show  $q_c(M) > 0$ . This is the most difficult part, for which we need to prove the following result.

**Claim 3** There exists  $q > 0$  such that  $\mathbf{u} \in \mathbb{G}_{M,q}$  implies  $\mathbf{u} = \mathbf{z}^M$ .

To disprove the presence of  $u_0$ , we shall use (4.3). In fact we will only use  $q \int u_0^2 \geq 2\beta_s \int u_0^2(u_1 - u_{-1})^2$ , from which it's easy to see  $u_0 = 0$  if  $q = 0$ . This is the argument used in [20]. For  $q > 0$ , however, whether  $u_0 = 0$  is not so obvious. Our proof of Claim 3 is based on the following lemma.

**Lemma 5.2.** *Given  $q \geq 0$ , if  $q_n \rightarrow q$  and  $\mathbf{u}^n \in \mathbb{G}_{M,q_n}$  is such that  $\mathbf{u}^n$  converges to some  $\mathbf{u} \in \mathbb{G}_{M,q}$  in  $\mathbb{B}$ , then the following assertions hold.*

(a) *There exists  $R > 0$  independent of  $n$  such that*

$$\frac{1}{2} \int (u_0^n)^2 \leq \int_{B(R)} (u_0^n)^2. \quad (5.1)$$

(b)  $\mathbf{u}^n \rightarrow \mathbf{u}$  *uniformly.*

We first prove Claim 3 by these two lemmas.

*Proof of Claim 3.* By Corollary 3.6, there exist a sequence  $q_n \rightarrow 0^+$  such that  $q_n \neq 0$  for each  $n$ , and a sequence  $\mathbf{u}^n \in \mathbb{G}_{M,q_n}$  such that  $\mathbf{u}^n \rightarrow \mathbf{z}^M$  in  $\mathbb{B}$ . Let  $R$  be as asserted in Assertion (a) of Lemma 5.2, and let  $k = \inf_{B(R)} (z_1^M - z_{-1}^M)$ . Note that  $k > 0$  by Remark 3.3. Now by Assertion (b) of Lemma 5.2,  $\mathbf{u}^n \rightarrow \mathbf{z}^M$  uniformly, and hence  $(u_1^n - u_{-1}^n) \geq k/2$  on  $B(R)$  for large  $n$ . From this fact and Assertion (a) we obtain

$$\begin{aligned} \int (u_0^n)^2 (u_1^n - u_{-1}^n)^2 &\geq \int_{B(R)} (u_0^n)^2 (u_1^n - u_{-1}^n)^2 \\ &\geq \frac{k^2}{4} \int_{B(R)} (u_0^n)^2 \\ &\geq \frac{k^2}{8} \int (u_0^n)^2 \end{aligned} \quad (5.2)$$

for  $n$  large enough. On the other hand, for any  $n$ , (4.3) implies

$$q_n \int (u_0^n)^2 \geq 2\beta_s \int (u_0^n)^2 (u_1^n - u_{-1}^n)^2. \quad (5.3)$$

Since  $q_n \rightarrow 0^+$ , (5.2) and (5.3) implies  $u_0^n$  must vanish for large  $n$ , which completes the proof.  $\square$

Now we prove Lemma 5.2.

*Proof of Lemma 5.2.* We first prove Assertion (b). The idea is that, if the GP system (2.2) for  $\mathbf{u}^n$  tends to that for  $\mathbf{u}$ , then uniform convergence can be obtained by the global boundedness result for elliptic operators. For this purpose, we need to show that the Lagrange multipliers for  $\mathbf{u}^n$ , denoted by  $\mu_n$  and  $\lambda_n$ , converge to those for  $\mathbf{u}$ , denoted by

$\mu$  and  $\lambda$  as before. This can be done as follows. Multiply (2.2a) by  $u_1$  and multiply (2.2c) by  $u_{-1}$ , and integrate, we obtain  $(\mu + j\lambda) \int u_j^2 = F_j(\mathbf{u}, q)$  for  $j = 1, -1$ , where

$$F_j(\mathbf{u}, q) = \int \left\{ |\nabla u_j|^2 + V u_j^2 + 2\beta_n |\mathbf{u}|^2 u_j^2 + 2\beta_s [u_0^2 u_j (u_j - u_{-j}) + u_j^2 (u_j^2 - u_{-j}^2)] + q u_j^2 \right\}.$$

Solve for  $\mu$  and  $\lambda$  we obtain

$$\begin{aligned} \mu &= [F_1(\mathbf{u}, q) / (\int u_1^2) + F_{-1}(\mathbf{u}, q) / \int u_{-1}^2] / 2 \\ \lambda &= [F_1(\mathbf{u}, q) / (\int u_1^2) - F_{-1}(\mathbf{u}, q) / \int u_{-1}^2] / 2. \end{aligned} \quad (5.4)$$

$\mu_n$  and  $\lambda_n$  can also be expressed by the above formulas, with  $\mathbf{u}$  replaced by  $\mathbf{u}^n$  and  $q$  replaced by  $q_n$ . Note that since we assume  $0 < M < 1$ , each  $\int (u_j^n)^2$  and  $\int u_j^2$  are nonzero for  $j = 1, -1$ . As a consequence,  $\mu_n \rightarrow \mu$  and  $\lambda_n \rightarrow \lambda$  follow the fact  $\mathbf{u}^n \rightarrow \mathbf{u}$  in  $\mathbb{B}$ .

Now let  $v_j^n = u_j^n - u_j$ . Subtract (2.2a) for  $\mathbf{u}$  from (2.2a) for  $\mathbf{u}^n$ , we obtain

$$\Delta v_1^n - V v_1^n = P_n + S(\mathbf{u}^n) - S(\mathbf{u}), \quad (5.5)$$

where

$$\begin{aligned} P_n &= -(\mu_n + \lambda_n - q_n) u_1^n + (\mu + \lambda - q) u_1, \\ S(\mathbf{u}) &= 2\beta_n |\mathbf{u}|^2 u_1 + 2\beta_s [u_0^2 (u_1 - u_{-1}) + u_1 (u_1^2 - u_{-1}^2)]. \end{aligned}$$

Apply global boundedness theorem for elliptic operators (see e.g. [10], Theorem 8.16) to (5.5), we have

$$\sup_{B(r)} |v_1^n| \leq \sup_{\partial B(r)} |v_1^n| + C \|P_n + S(\mathbf{u}^n) - S(\mathbf{u})\|_{L^2}, \quad (5.6)$$

where  $C > 0$  depends only on the radius  $r$  and  $\sup_{B(r)} V$ . Now since  $\mu_n \rightarrow \mu$ ,  $\lambda_n \rightarrow \lambda$ ,  $q_n \rightarrow q$ , and  $\mathbf{u}^n \rightarrow \mathbf{u}$  in  $\mathbb{B}$ , we see  $P_n \rightarrow 0$  in  $L^2$ , and also  $S(\mathbf{u}^n) - S(\mathbf{u}) \rightarrow 0$  in  $L^2$  since  $H^1$  is continuously embedded in  $L^6$ . On the other hand, also since  $\mu_n \rightarrow \mu$  and  $\lambda_n \rightarrow \lambda$ , by Lemma 3.12, we can find  $M_j(t)$  independent of  $n$  such that  $u_j$  and each  $u_j^n$  are bounded above by  $M_j(t) e^{-t|x|}$ . In particular, for any  $\varepsilon > 0$ , there exists  $r > 0$  such that

$$\sup_{|x| \geq r} |v_1^n(x)| \leq \varepsilon \quad (5.7)$$

for all  $n$ . Fix this  $r$  in (5.6) and let  $n \rightarrow \infty$ , we obtain

$$\limsup_{n \rightarrow \infty} \left( \sup_{x \in B(r)} |v_1^n(x)| \right) \leq \varepsilon. \quad (5.8)$$

From (5.7) and (5.8) we have  $\sup_{\mathbb{R}^3} |v_1^n| \leq 2\varepsilon$  for large  $n$ . Since  $\varepsilon > 0$  is arbitrary, we conclude that  $v_1^n \rightarrow 0$  uniformly. Similarly we have  $v_0^n$  and  $v_{-1}^n$  converge to zero uniformly, which completes the proof of Assertion (b).

Then for Assertion (a). As mentioned we have  $\mu_n \rightarrow \mu$  and hence  $\mu_n$  forms a bounded sequence, say  $\mu_n \leq C$  for some constant  $C > 0$ . Now multiply (2.2b) for  $\mathbf{u}^n$  by  $u_0^n$ , and then integrate, we obtain

$$\mu_n \int (u_0^n)^2 = \int \{ |\nabla u_0^n|^2 + V(u_0^n)^2 + 2\beta_n |\mathbf{u}^n|^2 (u_0^n)^2 + 2\beta_s (u_0^n)^2 (u_1^n - u_{-1}^n)^2 \},$$

which implies

$$\int V(u_0^n)^2 \leq \mu_n \int (u_0^n)^2 \leq C \int (u_0^n)^2. \quad (5.9)$$

On the other hand, by the assumption (A1), there exists  $R > 0$  such that  $V(x) \geq 2C$  for  $|x| > R$ , and hence

$$\int V(u_0^n)^2 \geq \int_{B(R)^c} V(u_0^n)^2 \geq 2C \int_{B(R)^c} (u_0^n)^2. \quad (5.10)$$

From (5.9) and (5.10), we obtain  $\int (u_0^n)^2 \geq 2 \int_{B(R)^c} (u_0^n)^2$ , which is equivalent to (5.1).  $\square$

Now we have completed the proof of Theorem 5.1. We remark that, however, it doesn't provide a good description of  $q_c(M)$ , even in a qualitative sense. Notably, we don't know why  $q_c$  should be a continuous increasing function of  $M$ , as is quite apparent from the numerical results. Nevertheless, one fact that is not quite clear numerically can be settled by our method. That is, as  $M \rightarrow 1^-$ , whether  $q_c(M)$  is tending to infinity or some finite number. The following complement of Theorem 5.1 says it's the latter that is the case.

**Theorem 5.3.** *There is a  $\bar{q} > 0$  such that if  $q > \bar{q}$ ,  $\mathbf{u} \in \mathbb{G}_{M,q}$  satisfies  $u_0 > 0$  for every  $M \in (0, 1)$ .*

*Proof.* Let's denote the left-hand side of (4.2) by  $L(M)$ , i.e.

$$L(M) = 4\beta_s \int z_1^M z_{-1}^M (z_1^M - z_{-1}^M) (\tau z_{-1}^M - z_1^M).$$

It suffices to show that  $L(M)$  is uniformly bounded for  $M \in (0, 1)$ . Note that

$$\begin{aligned} L(M) &\leq 4\beta_s \int z_1^M z_{-1}^M \cdot (z_1^M) \cdot (\tau z_{-1}^M) = 4\beta_s \tau \int (z_1^M)^2 (z_{-1}^M)^2 \\ &\leq 4\beta_s \tau \|z_1^M\|_{L^\infty}^2 \int (z_{-1}^M)^2 = 2\beta_s (1 + M) \|z_1^M\|_{L^\infty}^2. \end{aligned}$$

Thus it suffices to show that  $\|z_1^M\|_{L^\infty}$  is uniformly bounded. However, since  $\mathbf{z}^M$  is the unique element in  $\mathbb{G}_{M,0}$ , from Corollary 3.4 the map  $M \mapsto \mathbf{z}^M$  from  $[0, 1]$  into  $\mathbb{B}$  is continuous, and we can prove that  $M \mapsto z_1^M$  is also continuous from  $[0, 1]$  into  $L^\infty$  by imitating the proof of Assertion (b) of Lemma 5.2, which completes the proof.  $\square$

*Remark 5.1.* It might be a little surprising that, by the same argument, we have trouble to conclude that  $M \mapsto z_{-1}^M$  is also continuous from  $[0, 1]$  into  $L^\infty$ . Indeed, the problem only occurs at  $M = 1$ , where  $z_{-1}^M$  is equal to zero. See Section 6.2 for discussion.

## 5.2 Some characterizations of $q_c(M)$

In the following we also fix an  $M \in (0, 1)$ . Although our statement of Theorem 5.1 is a qualitative one, our proof does provide some quantitative information. For example, as the proof of Claim 1 says, (4.2) gives an upper bound of the value  $q$  for which  $\mathbf{z}^M \in \mathbb{G}_{M,q}$ , which means we have an upper bound of  $q_c(M)$  in terms of  $\mathbf{z}^M$ . Precisely, we have  $q_c(M) \leq U(M)$ , where

$$U(M) = \frac{1}{1+M} \left\{ 4\beta_s \int z_1^M z_{-1}^M (z_1^M - z_{-1}^M) (\tau z_{-1}^M - z_1^M) - \int \frac{\tau S(z_1^M, z_{-1}^M)}{(z_1^M)^2 + \tau (z_{-1}^M)^2} \right\}.$$

Similarly, (4.3) implies  $q_c(M) \geq \inf \mathcal{F}[\mathbf{u}]$ , where

$$\mathcal{F}[\mathbf{u}] = \frac{\beta_s \int u_0^2 (u_1 - u_{-1})^2 (2 + u_0^2 / (u_1 u_{-1})) + \int \sum_{j=1,-1} S(u_j, u_0) / u_j^2}{\int u_0^2},$$

and the infimum is taken over all  $\mathbf{u} \in \cup_{q \geq 0} \mathbb{G}_{M,q}$  such that  $u_0 > 0$ . Indeed, from Theorem 4.5, this  $\inf \mathcal{F}[\mathbf{u}]$  is equal to  $q_c(M)$ . To see this, for  $q > q_c(M)$  let  $\mathbf{u}^q$  be an element in  $\mathbb{G}_{M,q}$ , then  $u_0^q > 0$ . By Theorem 4.5 we have  $q = \mathcal{F}[\mathbf{u}^q]$ , and hence

$$q_c(M) = \lim_{q \rightarrow q_c(M)^+} q = \lim_{q \rightarrow q_c(M)^+} \mathcal{F}[\mathbf{u}^q] = \inf \mathcal{F}[\mathbf{u}]. \quad (5.11)$$

Of course this characterization is not of much use as to compute  $q_c(M)$ . In contrast, to obtain the upper bound  $U(M)$ , one needs only to find the 2C ground state  $\mathbf{z}^M$ , which really gives a great reduction in computation cost. To conclude this section, we explain that we can also modify  $U(M)$  to a characterization of  $q_c(M)$  as long as there is a sequence  $\mathbf{u}^n \in \mathbb{G}_{M,q_n}$ , where  $q_n \rightarrow q_c(M)^+$ , such that  $\mathbf{u}^n \rightarrow \mathbf{z}^M$  in  $\mathbb{B}$ . Before doing so, we remark that the existence of such sequence is left open in this paper, since we do not show that  $\mathbf{z}^M$  is the unique element in  $\mathbb{G}_{M,q_c(M)}$ . See the discussion on uniqueness in Section 6.1.

Now for  $q > q_c(M)$  and  $\mathbf{u} \in \mathbb{G}_{M,q}$ , consider  $\mathbf{u}(\delta)$  defined by

$$\begin{cases} u_1(\delta)^2 = (1 - \delta)u_1^2 \\ u_0(\delta)^2 = u_0^2 + \delta u_1^2 + \sigma \delta u_{-1}^2 \\ u_{-1}(\delta)^2 = (1 - \sigma \delta)u_{-1}^2. \end{cases}$$

Here  $\sigma = \sigma(\mathbf{u}) = (\int u_1^2)/(\int u_{-1}^2)$ . This  $\mathbf{u}(\delta)$  can be regarded as the same as that given in the proof of Lemma 4.1 except for  $u_0 > 0$ . In particular note that  $\sigma \rightarrow \tau = (1+M)/(1-M)$  as  $\int u_0^2 \rightarrow 0$ . One can check that such defined  $\mathbf{u}(\delta)$  is in  $\mathbb{A}_M$ . Follow the idea of proving Theorem 4.5, we will get the following equality.

**Theorem 5.4.** *Let  $M \in (0, 1)$  and  $q > q_c(M)$ .  $\mathbf{u} \in \mathbb{G}_{M,q}$  satisfies*

$$\begin{aligned} 4\beta_s \int u_1 u_{-1} (u_1 - u_{-1})(\sigma u_{-1} - u_1) + 2\beta_s \int u_0^2 (u_1 - u_{-1})(\sigma u_{-1} - u_1) \\ = q \int (u_1^2 + \sigma u_{-1}^2) + \int \frac{S(u_0, u_1) + \sigma S(u_0, u_{-1})}{u_0^2}. \end{aligned}$$

Now if we have  $q_n \rightarrow q_c(M)^+$  and  $\mathbf{u}^n \in \mathbb{G}_{M,q_n}$  such that  $\mathbf{u}^n \rightarrow \mathbf{z}^M$  in  $\mathbb{B}$ , by the above theorem we get the following characterization of  $q_c(M)$ :

$$\begin{aligned} q_c(M) = \frac{1}{1+M} \left\{ 4\beta_s \int z_1^M z_{-1}^M (z_1^M - z_{-1}^M)(\tau z_{-1}^M - z_1^M) \right. \\ \left. - \lim_{n \rightarrow \infty} \int \frac{S(u_0^n, u_1^n) + \sigma_n S(u_0^n, u_{-1}^n)}{(u_0^n)^2} \right\}, \end{aligned} \quad (5.12)$$

where  $\sigma_n = (\int (u_1^n)^2)/(\int (u_{-1}^n)^2)$ . It remains to show that (5.12) gives the upper bound  $U(M)$ . To see why (5.12) gives the upper bound  $U(M)$ , let  $\mathbf{f} = \nabla u_0/u_0$  (for general  $\mathbf{u} \in \mathbb{B}$  with  $u_0 > 0$ ), and we have

$$\begin{aligned} \frac{S(u_0, u_1) + \sigma S(u_0, u_{-1})}{u_0^2} &= |\nabla u_1 - u_1 \mathbf{f}|^2 + \sigma |\nabla u_{-1} - u_{-1} \mathbf{f}|^2 \\ &= (u_1^2 + \sigma u_{-1}^2) |\mathbf{f}|^2 - 2(u_1 \nabla u_1 + \sigma u_{-1} \nabla u_{-1}) \cdot \mathbf{f} + |\nabla u_1|^2 + \sigma |\nabla u_{-1}|^2 \\ &= (u_1^2 + \sigma u_{-1}^2) \left| \mathbf{f} - \frac{u_1 \nabla u_1 + \sigma u_{-1} \nabla u_{-1}}{u_1^2 + \sigma u_{-1}^2} \right|^2 + \frac{\sigma S(u_1, u_{-1})}{u_1^2 + \sigma u_{-1}^2} \\ &\geq \frac{\sigma S(u_1, u_{-1})}{u_1^2 + \sigma u_{-1}^2}. \end{aligned} \quad (5.13)$$

Thus, by choosing a subsequence  $\mathbf{u}^{n(k)}$  of  $\mathbf{u}^n$  so that  $\mathbf{u}^{n(k)} \rightarrow \mathbf{z}^M$  and  $\nabla \mathbf{u}^{n(k)} \rightarrow \nabla \mathbf{z}^M$  almost everywhere, we can apply Fatou's lemma to obtain

$$\lim_{k \rightarrow \infty} \int \frac{S(u_0^{n(k)}, u_1^{n(k)}) + \sigma_{n(k)} S(u_0^{n(k)}, u_{-1}^{n(k)})}{(u_0^{n(k)})^2} \geq \int \frac{\tau S(z_1^M, z_{-1}^M)}{(z_1^M)^2 + \tau (z_{-1}^M)^2}.$$

By substituting this inequality into (5.12) we find  $q_c(M) \leq U(M)$ .

## 6 Discussions and Open Problems

In this section we discuss some natural questions arising from this paper. They are categorized into three subsections.

## 6.1 Uniqueness

Uniqueness is a standard and prominent problem to be settled in variational problems. In this paper, although it's not essential, from time to time our presentation was plagued by the lack of it. For example, assume we have uniqueness, then we can simply use a symbol  $\mathbf{u}^{M,q}$  to denote the element in  $\mathbb{G}_{M,q}$ , and the wordy statements of Corollary 3.4 and Corollary 3.6 simply say that  $(M, q) \mapsto \mathbf{u}^{M,q}$  is a continuous map from  $[0, 1] \times [0, \infty)$  into  $\mathbb{B}$ . Nevertheless, we have mentioned in Remark 2.2 that our energy functional  $\mathcal{E}$  doesn't have the suitable convexity property due to the term  $2\beta_s u_0^2 (u_1 - u_{-1})^2$  appearing in  $H_s(\mathbf{u})$ . As to remedy this difficulty, there are two natural ideas:

- (a) Although  $\mathcal{E}$  is not convex on  $\mathbb{B}$ , it might be convex on a fixed  $\mathbb{A}_M$ , which is sufficient to prove uniqueness.
- (b) In this paper there is no assumption on the magnitude of  $\beta_s$ , while in practical spin-1 BECs (see references given in the introduction) it's very small compared to  $\beta_n$ , and hence  $\mathcal{E}_s$  contribute to a rather insignificant amount of the whole energy. If we are willing to take this into consideration, maybe the convexity of other parts will outweigh the nonconvexity of  $\mathcal{E}_s$ .

We are here to show that both ideas do not work. A counterexample is as follows. Let  $f, g, h$  be any three nonnegative functions in  $H^1 \cap L_V^2 \cap L^4$  such that 1)  $f, g$  and  $h$  are supported on disjoint sets, 2)  $\int (f^2 + g^2 + h^2) = 1$ , and 3)  $\int g^2 = \int h^2 > 0$  and  $\int (f^2 - g^2) = M$ . Then let  $\mathbf{u} = (f, g, h)$  and  $\mathbf{v} = (f, h, g)$ . We have  $\mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbb{A}_M$ , where  $w_j = (u_j^2 + v_j^2)^{1/2}$  as in the proof of Lemma 2.5. Let  $\Omega_f = \text{supp}(f)$ ,  $\Omega_g = \text{supp}(g)$  and  $\Omega_h = \text{supp}(h)$ , then it's easy to check that

$$\begin{aligned} \frac{1}{2}(\mathcal{E}[\mathbf{u}] + \mathcal{E}[\mathbf{v}]) - \mathcal{E}[\mathbf{w}] &= \frac{1}{2}(\mathcal{E}_s[\mathbf{u}] + \mathcal{E}_s[\mathbf{v}]) - \mathcal{E}_s[\mathbf{w}] \\ &= \beta_s \left( \int_{\Omega_f} + \int_{\Omega_g} + \int_{\Omega_h} \right) \left\{ \frac{1}{2}(H_s(\mathbf{u}) + H_s(\mathbf{v})) - H_s(\mathbf{w}) \right\} \\ &= \beta_s \left\{ \int_{\Omega_f} 0 + \int_{\Omega_g} -\frac{g^4}{4} + \int_{\Omega_h} -\frac{h^4}{4} \right\} < 0. \end{aligned}$$

Thus, no matter how small  $\beta_s$  is,  $\mathcal{E}$  doesn't have the desired convexity property on  $\mathbb{A}_M$ . Of course, the  $\mathbf{u}$  and  $\mathbf{v}$  above are far from being ground states, especially due to the assumption that the supports of the components are disjoint. We can go on to suspect  $\mathcal{E}$  might satisfy  $\frac{1}{2}(\mathcal{E}[\mathbf{u}] + \mathcal{E}[\mathbf{v}]) - \mathcal{E}[\mathbf{w}] \geq 0$  as long as  $\mathbf{u}$  and  $\mathbf{v}$  are "similar to" ground states. Anyway, uniqueness for our model, if holds, can not be obtained from the usual convexity argument. On the other hand, it's also not quite clear whether uniqueness holds from numerical simulations. The trickiest part lies on the bifurcation point. To have a better understanding of the problem, remember that the "nonuniqueness" point  $(M, q) = (0, 0)$  connects two boundary regimes which sharply contrast to each other: For

$M > 0$  and  $q = 0$ ,  $\mathbf{u} \in \mathbb{G}_{M,0}$  has  $u_0 = 0$ , while for  $q > 0$  and  $M = 0$ ,  $u_0$  is the only nonvanishing component of  $\mathbf{u} \in \mathbb{G}_{0,q}$ . It's observed in numerical simulations that such sharp contrast also occurs along the curve of bifurcation points  $(M, q_c(M))$ , so sharp that one is not easy to tell whether  $u_0$  shrinks to zero rapidly as  $q$  decreases to  $q_c(M)$ , or indeed there are both 2C ground state and 3C ground state at  $q_c(M)$ . In [19], the latter is claimed to be the case. However, in other simulations by using numerical continuation method (from not published private discussion. See [7] for related study of bifurcation with respect to  $\beta_n$  and  $\beta_s$ ), one can really track the changes of ground state from 3C profile to 2C profile as  $q$  decreases from a large number to zero, and it seems ground state is always unique (for  $(M, q) \neq (0, 0)$ ).

## 6.2 Uniform variations of ground states at boundary regimes

We have stated the bifurcation phenomenon in terms of varying  $q$  and fixed  $M$ . This choice is physically natural as the value of  $q$  can be tuned by modifying the applied magnetic field. From a mathematical point of view, however, we'd like to remark that this choice is in fact made intentionally. Somewhat unexpectedly at first sight, there are two difficulties to imitate the proof of Theorem 5.1 if we consider the bifurcation with varying  $M$  and fixed  $q$ . The first one is that we lack an analogue of Claim 2 in Section 5.1. Precisely, we do not know how to prove that if there is  $\mathbf{u} \in \mathbb{G}_{M,q}$  satisfying  $u_0 > 0$ , then every  $\mathbf{v} \in \mathbb{G}_{M',q}$  with  $M' < M$  must have  $v_0 > 0$ , or equivalently  $\mathbf{z}^M \in \mathbb{G}_{M,q}$  implies  $\mathbf{z}^{M'} \in \mathbb{G}_{M',q}$  for  $M' > M$ . As a consequence, we can't conclude that there exists a number  $M_c(q)$  which definitely separates the 2C regime and the 3C regime. The second problem, more fundamental, is that we are not sure whether the Lagrange multipliers will converge as  $M$  tends to  $1^-$  or  $0^+$ . Note that in either case  $\int u_{-1}^2 \rightarrow 0$  for  $\mathbf{u} \in \mathbb{G}_{M,q}$ , and we can not use the formula (5.4) directly. As a consequence, we can't obtain uniform convergence when  $M \rightarrow 1^-$  or  $0^+$  as in Lemma 5.2. Despite of this, we remark that in either situation it's known that the component which is not tending to zero does converge uniformly. For example, let  $M_n \rightarrow 1^-$  and  $\mathbf{u}^n \in \mathbb{G}_{M_n,q}$  converges in  $\mathbb{B}$  to the unique element in  $\mathbb{G}_{1,q}$ , which we denote by  $\mathbf{u}^\infty = (u_1^\infty, 0, 0)$ , then we also have  $u_1^n \rightarrow u_1^\infty$  uniformly. This is because anyway  $\mu_n + \lambda_n$  converges, and (2.2a) for  $\mathbf{u}^n$  tends to (2.2a) for  $\mathbf{u}^\infty$ . What left open is whether  $u_0^n$  and  $u_{-1}^n$  converge to zero uniformly. This lack of uniform convergence (of  $u_{-1}^n$  precisely) then prevents us from imitating the proof of Claim 3 to conclude that  $u_0^n = 0$  for large  $n$ . Similarly, when  $M \rightarrow 0^+$ , we only know  $u_0$  converges uniformly but not for  $u_1$  and  $u_{-1}$ . (Of course, this is sufficient to conclude that  $u_0 > 0$  when  $M$  is close to zero.) As we have mentioned in the remark after Theorem 5.3, such problem also occurs for  $\mathbf{z}^M$  when  $M \rightarrow 1^-$ , where  $z_{-1}^M$  converges to zero in  $\mathbb{B}$ , and we don't know if it converges uniformly.

### 6.3 Asymptotic behaviors at infinity

We are not sure whether  $\frac{d}{d\delta}\mathcal{E}[\mathbf{u}(\delta)]\big|_{\delta=0^+}$  exists for some constructions of redistributional perturbation  $\mathbf{u}(\delta)$ . An example is given by

$$\begin{cases} u_1(\delta)^2 = (1 - \delta)u_1^2 + \sigma\delta u_{-1}^2 \\ u_0(\delta)^2 = u_0^2 \\ u_{-1}(\delta)^2 = \delta u_1^2 + (1 - \sigma\delta)u_{-1}^2, \end{cases}$$

where assume  $\mathbf{u} \in \mathbb{G}_{M,q}$  is such that  $u_j > 0$  for each  $j$ , and  $\sigma = (\int u_1^2)/(\int u_{-1}^2)$ . It's easy to see  $\mathbf{u}(\delta) \in \mathbb{A}_M$ . Thus we have  $D(\mathbf{u}(\delta)) = D_{kin}(\mathbf{u}(\delta)) + D_s(\mathbf{u}(\delta)) \geq 0$ , but we are not able to deduce from it that  $\frac{d}{d\delta}\mathcal{E}_{kin}[\mathbf{u}(\delta)]\big|_{\delta=0^+} + \frac{d}{d\delta}\mathcal{E}_s[\mathbf{u}(\delta)]\big|_{\delta=0^+} \geq 0$  since we do not know if the derivatives exist. Indeed, if we differentiate them formally under the integral signs, we obtain

$$\int \left\{ \frac{\sigma S(u_1, u_{-1})}{u_1^2} + \frac{S(u_{-1}, u_1)}{u_{-1}^2} \right\} \leq 2\beta_s \int (u_1^2 - u_{-1}^2)(\sigma u_{-1}^2 - u_1^2) \left( \frac{u_0^2}{u_1 u_{-1}} + 2 \right), \quad (6.1)$$

while neither the left-hand side nor the right-hand side are obviously finite. Note that for the left-hand side of (6.1), we know the term  $S(u_1, u_{-1})/u_1^2 = |\nabla u_{-1} - (u_{-1}/u_1)\nabla u_1|^2$  is integrable since  $u_{-1} \leq u_1$ , and it's  $S(u_{-1}, u_1)/u_{-1}^2$  that causes trouble. The problem here is very similar to that mentioned in Remark 4.2. Roughly speaking, they are all due to the fact that we do not have a comparison of the asymptotic behaviors of different components of ground states. We remark that some numerical experiments show that  $u_0(x) < u_{-1}(x) < u_1(x)$  as  $|x|$  large. In fact it looks like  $u_0/u_{-1} \rightarrow 0$  and  $u_{-1}/u_1 \rightarrow 0$  as  $|x| \rightarrow \infty$ . If this can be proved, then the right-hand side of (6.1) is finite, and we can justify the differentiation above. Also, one can see that the problem mentioned in Remark 4.2 disappears, and Theorem 4.5 can be obtained from the GP system (2.2) without using Proposition 4.2.

## Appendix

We prove Lemma 2.3 in this appendix. For convenience we restate the assertion below.

**Lemma.** *Let  $\{\mathbf{u}^n\}$  be a sequence in  $\mathbb{B}_+$ . Suppose  $\mathcal{N}[\mathbf{u}^n] \rightarrow 1$ ,  $\mathcal{M}[\mathbf{u}^n] \rightarrow M$ , and  $\mathcal{E}[\mathbf{u}^n]$  is uniformly bounded in  $n$ , then  $\{\mathbf{u}^n\}$  has a subsequence  $\{\mathbf{u}^{n(k)}\}_{k=1}^\infty$  converging weakly to some  $\mathbf{u}^\infty \in \mathbb{A}$ , which satisfies  $\mathcal{E}[\mathbf{u}^\infty] \leq \liminf_{k \rightarrow \infty} \mathcal{E}[\mathbf{u}^{n(k)}]$ . If we assume further that  $\mathcal{E}[\mathbf{u}^n] \rightarrow E_g$ , then  $\mathbf{u}^\infty \in \mathbb{G}$ , and  $\mathbf{u}^{n(k)} \rightarrow \mathbf{u}^\infty$  in the norm of  $\mathbb{B}$ .*

*Proof.* Since the five parts  $\mathcal{E}_{kin}$ ,  $\mathcal{E}_{pot}$ , etc. are nonnegative functionals on  $\mathbb{B}$ , the uniform boundedness of  $\mathcal{E}[\mathbf{u}^n]$  implies that of the five parts, and hence  $\{\mathbf{u}^n\}$  is a bounded sequence in  $\mathbb{B}$ . Thus  $\{\mathbf{u}^n\}$  has a weakly convergent subsequence  $\{\mathbf{u}^{n(k)}\}_{k=1}^\infty$  in  $\mathbb{B}$ , of which we denote the weak limit by  $\mathbf{u}^\infty$ .

We first prove  $\mathbf{u}^\infty \in \mathbb{A}$ . Since  $\{\mathbf{u}^n\}$  is a bounded sequence,  $\int V|\mathbf{u}^{n(k)}|^2 \leq C$  for some  $C > 0$  independent of  $n$ . By the assumption (A1), for any  $\varepsilon > 0$ , there exists  $R_\varepsilon > 0$  such that  $V(x) \geq C/\varepsilon$  for  $|x| > R_\varepsilon$ . Thus we have

$$C \geq \int V|\mathbf{u}^{n(k)}|^2 \geq \int_{B(R_\varepsilon)^c} V|\mathbf{u}^{n(k)}|^2 \geq \frac{C}{\varepsilon} \int_{B(R_\varepsilon)^c} |\mathbf{u}^{n(k)}|^2,$$

and hence  $\int_{B(R_\varepsilon)^c} |\mathbf{u}^{n(k)}|^2 \leq \varepsilon$  for each  $k$ . In particular  $\int_{B(R_\varepsilon)^c} (u_j^{n(k)})^2 \leq \varepsilon$  for each  $k$  and  $j = 1, 0, -1$ . The weak convergence of  $\mathbf{u}^{n(k)}$  in  $(H^1(\mathbb{R}^3))^3$  implies  $u_j^{n(k)} \rightharpoonup u_j^\infty$  weakly in  $L^2(\mathbb{R}^3)$ , and  $u_j^{n(k)} \rightarrow u_j^\infty$  strongly in  $L^2(B(R_\varepsilon))$ . Hence we have

$$\begin{aligned} \int (u_j^\infty)^2 &\leq \liminf_{k \rightarrow \infty} \int (u_j^{n(k)})^2 \\ &\leq \limsup_{k \rightarrow \infty} \int (u_j^{n(k)})^2 \\ &= \limsup_{k \rightarrow \infty} \left( \int_{B(R_\varepsilon)^c} (u_j^{n(k)})^2 + \int_{B(R_\varepsilon)} (u_j^{n(k)})^2 \right) \\ &\leq \varepsilon + \int_{B(R_\varepsilon)} (u_j^\infty)^2 \leq \varepsilon + \int (u_j^\infty)^2, \end{aligned} \tag{6.2}$$

where the first inequality is due to the weak lower semi-continuity of a norm. Since  $\varepsilon > 0$  is arbitrary, the first and the second inequalities of (6.2) must be equalities, which imply

$$\lim_{k \rightarrow \infty} \int (u_j^{n(k)})^2 = \int (u_j^\infty)^2 \tag{6.3}$$

for  $j = 1, 0, -1$ , and hence  $\mathbf{u}^\infty \in \mathbb{A}$ .

Now since  $\mathbf{u}^\infty$  is the weak limit of  $\mathbf{u}^{n(k)}$ ,  $\mathcal{E}[\mathbf{u}^\infty] \leq \liminf \mathcal{E}[\mathbf{u}^{n(k)}]$  is a consequence of standard weak lower semi-continuity theorem. See e.g. Theorem 1.6 of [27]. Indeed, by the same theorem we have

$$\begin{aligned} \int |\nabla u_j^\infty|^2 &\leq \liminf_{k \rightarrow \infty} \int |\nabla u_j^{n(k)}|^2, \\ \int V(u_j^\infty)^2 &\leq \liminf_{k \rightarrow \infty} \int V(u_j^{n(k)})^2, \end{aligned}$$

and

$$\int f(u_1^\infty, u_0^\infty, u_{-1}^\infty) \leq \liminf_{k \rightarrow \infty} \int f(u_1^{n(k)}, u_0^{n(k)}, u_{-1}^{n(k)})$$

for every continuous function  $f : \mathbb{R}^3 \rightarrow [0, \infty)$ . In particular every parts of  $\mathcal{E}$  satisfies such lower-semicontinuity inequality. We claim that these  $\liminf$ 's are all limits and the

inequalities are all equalities provided  $\mathcal{E}[\mathbf{u}^{n(k)}] \rightarrow E_g$ . This is easily seen by assuming otherwise. For example assume  $\int |\nabla u_j^\infty|^2 < \limsup \int |\nabla u_j^{n(k)}|^2$  for some  $j$ . Then we obtain

$$E_g = \lim_{k \rightarrow \infty} \mathcal{E}[\mathbf{u}^{n(k)}] > \mathcal{E}[\mathbf{u}^\infty],$$

contradicting to the fact  $\mathbf{u}^\infty \in \mathbb{A}$ . Thus the claim is true. This fact together with (6.3) imply  $\|u_j^{n(k)}\|_{H^1} \rightarrow \|u_j^\infty\|_{H^1}$ . Now since  $H^1$  is reflexive,  $\mathbf{u}^{n(k)} \rightharpoonup \mathbf{u}^\infty$  weakly in  $H^1$  and  $\|u_j^{n(k)}\|_{H^1} \rightarrow \|u_j^\infty\|_{H^1}$  implies  $\mathbf{u}^{n(k)} \rightarrow \mathbf{u}^\infty$  strongly in  $H^1$ . Similarly we can prove  $\mathbf{u}^{n(k)} \rightarrow \mathbf{u}^\infty$  in  $L_V^2$  and in  $L^4$ .  $\square$

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