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A KINETIC ENERGY REDUCTION TECHNIQUE AND CHARACTERIZATIONS OF THE GROUND STATES OF SPIN-1 BOSE-EINSTEIN CONDENSATES

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Abstract. We justify some characterizations of the ground states of spin-1 Bose-Einstein condensates exhibited from numerical simulations. For ferromagnetic systems, we show the validity of the single-mode approximation (SMA). For an antiferromagnetic system with nonzero magnetization, we prove the vanishing of the $m_F = 0$ component. In the end of the paper some remaining degenerate situations are also discussed. The proofs of the main results are all based on a simple observation, that a redistribution of masses among different components will reduce the kinetic energy.

1. **Introduction.** At ultra low temperature, massive bosons could occupy the same lowest-energy state and form the so-called Bose-Einstein condensates (BECs). This phenomenon was predicted by Bose and Einstein in 1925, and was first realized on several alkali atomic gases in 1995 by laser cooling technique [1, 7, 11]. In early experiments, the atoms were confined in magnetic traps. In this situation the spin degrees of freedom are frozen. Through the mean-field approximation the system is then described by a scalar wave function, which satisfies the Gross-Pitaevskii (GP) equation [10, 15, 24]. In contrast, in an optically trapped atomic BEC all hyperfine spin states can be active simultaneously, and a spin-F BEC is then described by a vector wave function $\Psi = (\psi_F, \psi_{F-1}, \cdots, \psi_{-F})^T$, where the j-th component corresponds to the $m_F = j$ hyperfine state [27, 28, 22, 4, 14]. The theory of such spinor BEC was first developed independently by several groups [23, 16, 18]. After these early studies, spinor BEC has become an area of great research interest.

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1.1. **Mathematical model for spin-1 BEC.** For a spin-1 BEC, the vector wave function $\Psi = (\psi_1, \psi_0, \psi_{-1})^T$ satisfies a generalized GP equation:

$$i\hbar\partial_t\Psi = \frac{\delta E}{\delta \Psi^*}, \tag{1}$$

where the Hamiltonian is given by

$$E[\Psi] := \int_D \left\{ \frac{\hbar^2}{2m_a}\sum_j |\nabla\psi_j|^2 + V(x)|\Psi|^2 + \frac{c_n}{2}|\Psi|^4 + \frac{c_s}{2}|\Psi^* S\Psi|^2 \right\} dx.$$

Here D is a domain in $\mathbb{R}^d$, $\hbar$ is the reduced Planck constant, m_a is the atomic mass, V is a locally bounded real-valued function representing the trap potential, Ψ^* is the Hermitian of Ψ, and $S = (S_x, S_y, S_z)$ is the triple of spin-1 Pauli matrices:

$$S_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},\ S_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},\ S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

So $\Psi^* S\Psi$ denotes the vector $(\Psi^* S_x\Psi, \Psi^* S_y\Psi, \Psi^* S_z\Psi)$. Also note that $|\Psi|$ denotes the Euclidean length $(\sum_j |\psi_j|^2)^{1/2}$, and similiarly for $|\nabla\psi_j|$ and $|\Psi^* S\Psi|$. The parameters c_n and c_s are real constants given by

$$c_n = \frac{4\pi\hbar^2}{3m_a}(a_0 + 2a_2),\ c_s = \frac{4\pi\hbar^2}{3m_a}(-a_0 + a_2),$$

where a_0 and a_2 are respectively the s-wave scattering lengths for scattering channels of total hyperfine spin zero and spin two. The parameter c_n characterizes the spin-independent interaction, and the parameter c_s characterizes the spin-exchange interaction. For $c_n < 0$ (resp. $c_n > 0$), the spin-independent interaction is attractive (resp. repulsive). For $c_s < 0$ (resp. $c_s > 0$), the spin-exchange interaction is ferromagnetic (resp. antiferromagnetic). Typical examples of ferromagnetic and antiferromagnetic systems are ^{87}Rb and ^{23}Na condensates.

The generalized GP equation (1) implies two conserved quantities:

$$\text{(C1)} \qquad \int_D |\Psi|^2 = N,$$

$$\text{(C2)} \qquad \int_D \left(|\psi_1|^2 - |\psi_{-1}|^2\right) = M,$$

where N is the total number of atoms and M is the total magnetization. For the system to be nontrivial, we assume $N > 0$. We also assume $|M| < N$ (note that obviously $|M| \le N$), for if $|M| = N$ the system reduces to a single component BEC, which is a trivial case for all considerations in this work. Now we say Ψ is a ground state if it is a minimizer of E under the above two constraints.

1.2. **Innovation and organization.** In researches concerning ground states of spin-1 BEC, the following ansatz was often adopted:

$$\psi_j = \gamma_j\psi \quad \text{for each} \quad j, \tag{2}$$

where γ_j are constants and ψ is a function independent of j. This is called the single-mode approximation (SMA) in the physics literature [18, 13, 26, 17, 25, 12]. It has been found [29] from numerical simulations that ground states obey the SMA exactly for ferromagnetic systems (and does not in general for antiferromagnetic ones), and hence can effectively be characterized as one-component systems. The first goal of this paper is to analytically confirm this observation. On the other hand, for

antiferromagnetic systems, we will show that $\psi_0 \equiv 0$[1] when $M \neq 0$, another well-known phenomenon from numerical simulations [3, 9] not being rigorously proved before. For the degenerate case $M = 0$, however, the SMA is again valid while ground states are not unique, and ψ_0 does not necessarily vanish. It's interesting that although the two phenomena (SMA and vanishing of ψ_0) look quite irrelevant to each other, they can be proved by the same simple principle, that a redistribution of masses between different components will decrease the kinetic energy.

The paper is organized as follows. Section 2 is the preliminary, where we reformulate the mathematical model more precisely, and then provide a result of maximum principle which is crucial in justifying the expected characterizations. In Section 2.2 the idea of mass redistribution is introduced. Sections 3 and 4 treat respectively the ferromagnetic and antiferromagnetic systems.

2. **Preliminary.** For notational simplicity, let's redefine

$$E[\Psi] = \int_D \left\{ \sum_j |\nabla \psi_j|^2 + V|\Psi|^2 + c_n|\Psi|^4 + c_s|\Psi^* S \Psi|^2 \right\}.$$

This causes no loss of generality for the phenomena we are going to investigate. The admissible class is

$$\mathcal{C} = \left\{ \Psi \in \left(H^1(D) \cap L^4(D) \cap L^2(D, V dx)\right)^3 \;\middle|\; \Psi \text{ satisfies (C1) and (C2)} \right\},$$

where $L^2(D, V dx)$ consists of all functions f such that $\int_D V|f|^2 < \infty$. Let $\mathbf{u}$ denotes (u_1, u_0, u_{-1}). We also define

$$\mathcal{A} = \{\mathbf{u} \in \mathcal{C} \mid u_j \geq 0 \text{ for each } j\};$$
$$\mathcal{A}_1 = \{\mathbf{u} \in \mathcal{A} \mid \mathbf{u} = (\gamma_1 f, \gamma_0 f, \gamma_{-1} f) \text{ for some constants } \gamma_j \text{ and some function } f\};$$
$$\mathcal{A}_2 = \{\mathbf{u} \in \mathcal{A} \mid u_0 \equiv 0\}.$$

Let's also use $\boldsymbol{\gamma}$ to denote $(\gamma_1, \gamma_0, \gamma_{-1})$, so that $(\gamma_1 f, \gamma_0 f, \gamma_{-1} f)$ can be abbreviated as $\boldsymbol{\gamma} f$.

In Section 2.1, we introduce a common reduction which asserts that to study ground states we can simply consider $\mathcal{A}$ instead of $\mathcal{C}$. Indeed, $\mathcal{A}$ consists just the amplitudes of elements in $\mathcal{C}$. And $\mathcal{A}_1$ (resp. $\mathcal{A}_2$) corresponds to the set of all elements obeying the SMA (resp. with vanishing zeroth components). For the moment, we do not consider any boundary condition for simplicity. See the remark after Theorem 3.1.

2.1. **Reduction from $\mathcal{C}$ to $\mathcal{A}$.** Given $\Psi \in \mathcal{C}$. Let $u_j e^{i\theta_j}$ be the polar form of ψ_j for each j. Then, by formally[2] differentiating the θ_j's, it's easy to check that

$$\begin{aligned} E[\Psi] = \int_D \Bigg\{ & \sum_j (|\nabla u_j|^2 + u_j^2 |\nabla \theta_j|^2) + V|\mathbf{u}|^2 + c_n|\mathbf{u}|^4 \\ & + c_s \Big[2u_0^2 \big(u_1^2 + u_{-1}^2 + 2u_1 u_{-1} \cos(\theta_1 - 2\theta_0 + \theta_{-1})\big)^2 + (u_1^2 - u_{-1}^2)^2 \Big] \Bigg\}. \end{aligned} \tag{3}$$

[1] We use "$f \equiv g$" to stress f is "identically" equal to g. We shall also usually only use "$=$" for equalities of functions later on, possibly in the sense of almost everywhere. There is no true point to distinguish them in this paper.

[2] The differentiation is formal since the fact that $\psi_j \in H^1$ alone doesn't imply we can choose θ_j to be also of class H^1. This is nevertheless possible by some "lifting" theorem. [5, 6]

For Ψ to be a ground state, we thus require the following:

$$\text{The } \theta_j\text{'s are constants and } \cos(\theta_1 - 2\theta_0 + \theta_{-1}) = \pm 1 \text{ for } c_s \lessgtr 0. \tag{4}$$

And then

$$E[\Psi] = \int_D \left\{ \sum_j |\nabla u_j|^2 + V|\mathbf{u}|^2 + c_n|\mathbf{u}|^4 + c_s\left[2u_0^2(u_1 \pm u_{-1})^2 + (u_1^2 - u_{-1}^2)^2\right]\right\}, \tag{5}$$

where the plus-minus sign $\pm$ corresponds to $c_s \lessgtr 0$.

Let's now define $\mathbb{E} : \mathcal{A} \to \mathbb{R}$, $\mathbb{E}[\mathbf{u}]$ is given by the right-hand side of (5). We use $\mathcal{G}$ to denote the set of all minimizers of $\mathbb{E}$ over $\mathcal{A}$. We will not rigorously establish a correspondence between ground states and elements in $\mathcal{G}$. For example, we will not justify the validity of the differentiation of the θ_j's in (3). Also note that if some component of a ground state Ψ vanishes, then (4) needs not be satisfied. Despite these problems, we claim that the assertion "every ground state obeys the SMA (2)" does be equivalent to "every element in $\mathcal{G}$ lies in $\mathcal{A}_1$." Similarly, the assertion that "every ground state Ψ has $\psi_0 \equiv 0$" is equivalent to "every $\mathbf{u}$ in $\mathcal{G}$ lies in $\mathcal{A}_2$." We shall omit the proofs of these facts. (See [21].) Without loss of generality, we henceforth consider $\mathbb{E}$ and $\mathcal{G}$ instead of the original model.

For convenience let's use H to denote the integrand of $\mathbb{E}$, i.e. $\mathbb{E}[\mathbf{u}] = \int_D H(\mathbf{u})$. We also write $H = H_1 + H_2$, where

$$H_1(\mathbf{u}) = \sum_j |\nabla u_j|^2 + c_s\left[2u_0^2(u_1 \pm u_{-1})^2 + (u_1^2 - u_{-1}^2)^2\right],$$
$$H_2(\mathbf{u}) = V|\mathbf{u}|^2 + c_n|\mathbf{u}|^4.$$

This splitting of H is only for convenience of later discussion.

The Euler-Lagrange system for $\mathbf{u} \in \mathcal{G}$ is given by the following coupled Gross-Pitaevskii equations:

$$\begin{cases} (\mu + \lambda)u_1 = \mathcal{L}u_1 + 2c_s\left[u_0^2(u_1 \pm u_{-1}) + u_1(u_1^2 - u_{-1}^2)\right] \\ \mu u_0 = \mathcal{L}u_0 + 2c_s u_0(u_1 \pm u_{-1})^2 \\ (\mu - \lambda)u_{-1} = \mathcal{L}u_{-1} + 2c_s\left[u_0^2(u_{-1} \pm u_1) + u_{-1}(u_{-1}^2 - u_1^2)\right], \end{cases} \tag{6}$$

where $\mathcal{L} = -\Delta + V + 2c_n|\mathbf{u}|^2$, and λ and μ are the Lagrange multipliers induced by the constraints (C1) and (C2). We remark that in this paper we do not involve ourselves in the problem of existence. To best illustrate the simplicity of our method, we just assume there is a ground state. (See [20, 8, 2] for related concerns of existence problem). Also note that $\mathbf{u} \in \mathcal{G}$ is continuously differentiable by standard regularity theorem.

The following lemma will be crucial in our characterizations of ground states.

Lemma 2.1. *If $\mathbf{u} \in \mathcal{G}$, then for each j, either $u_j \equiv 0$ or $u_j > 0$ on all of D.*

Proof. Let K be a compact subset of D. By subtracting respectively $Q_j u_j$, $j = 1, 0, -1$, from the three equations in (6) with large enough constants Q_j, and using the assumption $u_j \geq 0$, it's easy to verify that each u_j satisfies

$$\Delta u_j + h_j u_j \leq 0$$

for some function h_j which is non-positive on K. Thus either $u_j > 0$ or $u_j \equiv 0$ on K by the strong maximum principle. Since $K \subset D$ is arbitrary, the assertion of the lemma holds. □

2.2. **A kinetic-energy-reducing redistribution.** Consider an n-tuple of nonnegative functions $\mathbf{f} = (f_1, f_2, ..., f_n) \in (H^1(D))^n$. Let $g = |\mathbf{f}|$. It's well-known (see e.g. [19], Theorem 7.8) that $|\nabla g|^2 \le \sum_k |\nabla f_k|^2$. In fact,

$$\sum_k |\nabla f_k|^2 - |\nabla g|^2 = \begin{cases} \dfrac{1}{g^2} \displaystyle\sum_{j<k} |f_j \nabla f_k - f_k \nabla f_j|^2 & \text{on where } g > 0 \\ 0 & \text{on where } g = 0. \end{cases} \tag{7}$$

This convexity inequality for gradients has a simple while interesting generalization, when $f_1^2, f_2^2, \dots, f_n^2$ do not sum to a single g^2, but instead are redistributed into multiple parts. To be precise, we give the following definition.

Definition 2.2. Let $\mathbf{f}$ be as above, and let $\mathbf{g} = (g_1, g_2, ..., g_m)$ be an m-tuple of nonnegative functions. We say $\mathbf{g}$ is a square redistribution of $\mathbf{f}$ if

$$g_\ell^2 = \sum_{k=1}^n a_{\ell k} f_k^2 \quad \text{for} \quad \ell = 1, 2, \dots, m, \tag{8}$$

where $a_{\ell k}$ are constants, $a_{\ell k} \ge 0$, and $\sum_{\ell=1}^m a_{\ell k} = 1$ for each $k = 1, 2, \dots, n$.

Note that $g = |\mathbf{f}|$ is the only square redistribution of $\mathbf{f}$ for $m = 1$. In general we have the following result.

Theorem 2.3. *For any square redistribution* $\mathbf{g}$ *of* $\mathbf{f}$ *as in* Definition 2.2*, we have*

(a) $|\mathbf{g}| = |\mathbf{f}|$,

(b) $\sum_{\ell=1}^m |\nabla g_\ell|^2 \le \sum_{k=1}^n |\nabla f_k|^2$.

Proof. (a) follows by summing (8) over $\ell = 1, 2, \dots, m$. For fixed ℓ, apply the convexity inequality for gradients to the vector $(\sqrt{a_{\ell 1}} f_1, \sqrt{a_{\ell 2}} f_2, \dots, \sqrt{a_{\ell k}} f_k)$, we obtain

$$|\nabla g_\ell|^2 \le \sum_{k=1}^n a_{\ell k} |\nabla f_k|^2.$$

And (b) follows by summing this inequality over $\ell = 1, 2, \dots, m$. □

Remark. We can naturally generalize the idea to p-th power redistribution, which may be useful in studying systems with p-Laplacian terms.

To save notation, in the following we shall omit the adjective "square" and simply say "redistribution". Since the square of the amplitude of a wave function represents the distribution of its mass density, a redistribution of $\mathbf{u} \in \mathcal{A}$ means a redistribution of the masses between its three components. If $\mathbf{u} \in \mathcal{A}$ and $\mathbf{v} = (v_1, v_0, v_{-1})$ is a redistribution of $\mathbf{u}$, Theorem 2.3 (a) says the shapes of their total mass distribution are the same. In particular, $\mathbf{v}$ satisfies the first constraint (C1), and $H_2(\mathbf{v}) = H_2(\mathbf{u})$. These facts together with (b), which causes a reduction of the kinetic energy, allow us to give a simple and unified approach to our problems.

3. **Ferromagnetic systems.** In this section we assume $c_s < 0$, and the goal is to prove the validity of SMA, that is $\mathcal{G} \subset \mathcal{A}_1$. The idea is to find, for $\mathbf{u} \in \mathcal{A}$, a redistribution of $\mathbf{u}$ in $\mathcal{A}_1$ which has no larger energy than $\mathbf{u}$, and then try to conclude that $\mathbf{u}$ must itself be the redistributed element provided $\mathbf{u} \in \mathcal{G}$.

Now given any $\mathbf{u} \in \mathcal{A}$. It's easy to see that a redistribution of $\mathbf{u}$ lies in $\mathcal{A}_1$ if and only if it can be expressed as $\boldsymbol{\gamma}|\mathbf{u}|$, where $\boldsymbol{\gamma} = (\gamma_1, \gamma_0, \gamma_{-1})$ is a triple of nonnegative constants satisfying

$$\begin{cases} \gamma_1^2 + \gamma_0^2 + \gamma_{-1}^2 = 1 \\ \gamma_1^2 - \gamma_{-1}^2 = M/N. \end{cases} \tag{9}$$

Let Γ denote the set containing all such $\boldsymbol{\gamma}$:

$$\Gamma := \left\{ \boldsymbol{\gamma} \in \mathbb{R}^3 \;\middle|\; \gamma_j \geq 0 \text{ for each } j,\ \boldsymbol{\gamma} \text{ satisfies (9)} \right\}.$$

Then

$$H_1(\boldsymbol{\gamma}|\mathbf{u}|) = |\nabla|\mathbf{u}||^2 + c_s P(\boldsymbol{\gamma})|\mathbf{u}|^4,$$

where

$$P(\boldsymbol{\gamma}) = 2\gamma_0^2(\gamma_1 + \gamma_{-1})^2 + \frac{M^2}{N^2}.$$

For the redistributed $\boldsymbol{\gamma}|\mathbf{u}|$ to have no larger energy than $\mathbf{u}$, the best candidate is obviously obtained by maximizing $P(\boldsymbol{\gamma})$. It's easy to check that

$$\max_{\boldsymbol{\gamma} \in \Gamma} P(\boldsymbol{\gamma}) = P(\boldsymbol{\gamma}^\star) = 1,$$

where the maximizer $\boldsymbol{\gamma}^\star = (\gamma_1^\star, \gamma_0^\star, \gamma_{-1}^\star)$ is uniquely given by

$$\gamma_1^\star = \frac{1}{2}\left(1 + \frac{M}{N}\right),\ \gamma_0^\star = \sqrt{\frac{1}{2}\left(1 - \frac{M^2}{N^2}\right)},\ \text{and } \gamma_{-1}^\star = \frac{1}{2}\left(1 - \frac{M}{N}\right).$$

We can now state our main theorem of this section.

Theorem 3.1. *Assume $c_s < 0$. If $\mathbf{u} \in \mathcal{G}$, then $\mathbf{u} = \boldsymbol{\gamma}^\star|\mathbf{u}|$.*

Proof. Since $\boldsymbol{\gamma}^\star|\mathbf{u}|$ is a redistribution of $\mathbf{u}$, $H_2(\mathbf{u}) = H_2(\boldsymbol{\gamma}^\star|\mathbf{u}|)$. Hence

$$H(\mathbf{u}) - H(\boldsymbol{\gamma}^\star|\mathbf{u}|) = H_1(\mathbf{u}) - H_1(\boldsymbol{\gamma}^\star|\mathbf{u}|) =: D_k + D_s,$$

where

$$D_k = \sum_j |\nabla u_j|^2 - |\nabla|\mathbf{u}||^2 \geq 0$$

by (7), and

$$D_s = c_s\left[2u_0^2(u_1 + u_{-1})^2 + (u_1^2 - u_{-1}^2)^2\right] - c_s|\mathbf{u}|^4 = -c_s(u_0^2 - 2u_1u_{-1})^2 \geq 0.$$

However, $\mathbf{u} \in \mathcal{G}$, thus we must have $D_k = D_s = 0$. From (7), this occurs if and only if

$$u_j \nabla u_k - u_k \nabla u_j = 0 \quad \text{for} \quad j \neq k\,; \tag{10}$$

$$u_0^2 - 2u_1u_{-1} = 0. \tag{11}$$

Since we assume the total number of atoms $N > 0$, from Lemma 2.1, at least one u_j is strictly positive in D. Assume $u_1 > 0$ on D, then (10) implies

$$\nabla\left(u_0/u_1\right) = \nabla\left(u_{-1}/u_1\right) = 0. \tag{12}$$

Since D is connected, (12) implies u_0 and u_{-1} are both constant multiples of u_1. This shows $\mathbf{u} \in \mathcal{A}_1$. The same conclusion holds obviously if $u_0 > 0$ or $u_{-1} > 0$. That $\mathbf{u}$ must be $\boldsymbol{\gamma}^\star|\mathbf{u}|$ then follows either by (11) or by the fact that $\boldsymbol{\gamma}^\star$ is the unique maximizer of P over Γ. □

Remark. We can add more assumptions in the definition of $\mathcal{A}$ for Theorem 3.1 to hold. The only thing we need to take care is that we need $\boldsymbol{\gamma}^\star|\mathbf{u}| \in \mathcal{A}$ whenever $\mathbf{u} \in \mathcal{G}$, so that $\mathbb{E}[\mathbf{u}] \le \mathbb{E}[\boldsymbol{\gamma}^\star|\mathbf{u}|]$ is not violated. For example, we can consider a homogeneous boundary condition (e.g. homogeneous Dirichlet or Neumann boundary condition) for $\mathbf{u} \in \mathcal{A}$, since then $\boldsymbol{\gamma}^\star|\mathbf{u}|$ also satisfies the same condition.

Theorem 3.1 implies that searching for ground states of ferromagnetic spin-1 BEC can be reduced to a single-component minimization problem. Precisely, define the single-component admissible class

$$\begin{aligned}\mathcal{A}^s &= \{|\mathbf{u}| \mid \mathbf{u} \in \mathcal{A}\} \\ &= \left\{u \in H^1(D) \cap L^4(D) \cap L^2(D, V\,dx) \;\middle|\; u \ge 0,\ \textstyle\int_D u^2 = N\right\},\end{aligned} \tag{13}$$

and define

$$\begin{aligned}\mathbb{E}^s[u] &= \textstyle\int_D \left\{|\nabla u|^2 + Vu^2 + (c_n + c_s)u^4\right\} \quad \text{for} \quad u \in \mathcal{A}^s, \\ \mathcal{G}^s &= \{u \in \mathcal{A}^s \mid \mathbb{E}^s[u] = \min\nolimits_{v \in \mathcal{A}^s} \mathbb{E}^s[v]\}.\end{aligned}$$

We have the following characterization.

Corollary. $\mathcal{G} = \{\boldsymbol{\gamma}^\star u \mid u \in \mathcal{G}^s\}$.

Proof. If $\mathbf{u} \in \mathcal{G}$, then $\mathbf{u} = \boldsymbol{\gamma}^\star|\mathbf{u}|$ by Theorem 3.1. To see $|\mathbf{u}| \in \mathcal{G}^s$, note that

$$\mathbb{E}^s[|\mathbf{u}|] = \mathbb{E}[\boldsymbol{\gamma}^\star|\mathbf{u}|] \le \mathbb{E}[\boldsymbol{\gamma}^\star v] = \mathbb{E}^s[v]$$

for every $v \in \mathcal{A}^s$. Conversely if $u \in \mathcal{G}^s$, we want to show $\boldsymbol{\gamma}^\star u \in \mathcal{G}$. This is true since

$$\mathbb{E}[\boldsymbol{\gamma}^\star u] = \mathbb{E}^s[u] \le \mathbb{E}^s[|\mathbf{v}|] = \mathbb{E}[\boldsymbol{\gamma}^\star|\mathbf{v}|] \le \mathbb{E}[\mathbf{v}]$$

for every $\mathbf{v} \in \mathcal{A}$. □

4. Antiferromagnetic systems and some degenerate cases.

The main focus of this section is the phenomenon $u_0 \equiv 0$. After justifying it in Section 4.1, some degenerate situations are also discussed in Section 4.2.

4.1. Justification of the vanishing phenomenon.

Assume $c_s > 0$ in this subsection. We want to show that any ground state must have a vanishing zeroth component. Similar to the approach in the previous section, we want to find an appropriate redistribution $\widetilde{\mathbf{u}}$ of $\mathbf{u} \in \mathcal{A}$ so that $\widetilde{\mathbf{u}} \in \mathcal{A}_2$ and $\mathbb{E}[\widetilde{\mathbf{u}}] \le \mathbb{E}[\mathbf{u}]$. Now, not as before, the assumption $\widetilde{\mathbf{u}} \in \mathcal{A}_2$ alone doesn't give rise to a definite hint for what $\widetilde{\mathbf{u}}$ should be. In view that such $\widetilde{\mathbf{u}}$ satisfies $|\widetilde{\mathbf{u}}| = |\mathbf{u}|$ and hence (C1), as a guess, we try just imposing the additional assumption that $\widetilde{\mathbf{u}}$ also satisfies

$$\widetilde{u}_1^2 - \widetilde{u}_{-1}^2 = u_1^2 - u_{-1}^2,$$

so that (C2) is also satisfied by $\widetilde{\mathbf{u}}$ automatically. This results in only one possibility, that is

$$\widetilde{u}_j = \sqrt{u_j^2 + \frac{u_0^2}{2}} \quad \text{for} \quad j = 1, -1. \tag{14}$$

It's fortunate that it works.

Theorem 4.1. *Assume $c_s > 0$ and $M \neq 0$, then $\mathbf{u} \in \mathcal{G}$ implies $u_0 = 0$.*

Proof. For $\mathbf{u} \in \mathcal{A}$, let $\widetilde{\mathbf{u}} \in \mathcal{A}_2$ be its redistribution defined by (14). Then

$$H(\mathbf{u}) - H(\widetilde{\mathbf{u}}) = D_k + D_s,$$

where

$$D_k = \sum_j |\nabla u_j|^2 - \sum_j |\nabla \widetilde{u}_j|^2 \geq 0$$

by Theorem 2.3 (b), and

$$D_s = 2c_s u_0^2 (u_1 - u_{-1})^2 \geq 0.$$

by direct computation. Assume $\mathbf{u} \in \mathcal{G}$, then we must have

$$u_0^2 (u_1 - u_{-1})^2 = 0.$$

(That $D_k = 0$ is also true but is not needed here.) By Lemma 2.1, either $u_0 \equiv 0$ or $u_1 \equiv u_{-1}$. However since we assume $M \neq 0$, we cannot have $u_1 \equiv u_{-1}$, and the assertion follows. □

4.2. **Some degenerate situations.** The requirement $M \neq 0$ in Theorem 4.1 is necessary. In fact, for $M = 0$, SMA is again valid while ground states are not unique, and $u_0 \equiv 0$ is not necessarily the case. Precisely, consider the minimization problem (recall that $\mathcal{A}^s$ is defined by (13))

$$\min_{v \in \mathcal{A}_s} \int_D \left\{ |\nabla v|^2 + V v^2 + c_n v^4 \right\}. \tag{15}$$

We have the following characterization.

Proposition 4.2. *If $c_s > 0, M = 0$ or $c_s = 0$, then*

$$\mathcal{G} = \left\{ \left(t, \sqrt{1-2t^2}, t\right) u \;\middle|\; 0 \leq t \leq 1/\sqrt{2},\ u \text{ is a minimizer of (15)} \right\}.$$

Proof. Note that since $M = 0$, from (9), $\boldsymbol{\gamma} \in \Gamma$ implies

$$\boldsymbol{\gamma} = \left(t, \sqrt{1-2t^2}, t\right) \quad \text{for some} \quad 0 \leq t \leq 1/\sqrt{2}.$$

Now it's easy to see that for any $\mathbf{u} \in \mathcal{A}$ and $\boldsymbol{\gamma} \in \Gamma$ we have

$$H(\boldsymbol{\gamma}|\mathbf{u}|) = |\nabla |\mathbf{u}||^2 + V|\mathbf{u}|^2 + c_n |\mathbf{u}|^4.$$

Thus, $H(\boldsymbol{\gamma}|\mathbf{u}|)$ is independent of $\boldsymbol{\gamma} \in \Gamma$, and $H(\boldsymbol{\gamma}|\mathbf{u}|) \leq H(\mathbf{u})$ obviously. The proof that $\mathbf{u} \in \mathcal{G}$ implies $\mathbf{u}$ must be one of the $\boldsymbol{\gamma}|\mathbf{u}|$ is much the same as in the proof of Theorem 3.1, and we omit it. □

In contrast to the above theorem, SMA is almost never the case when $M \neq 0$.

Proposition 4.3. *Assume $c_s > 0$ and $M \neq 0$, then $\mathbf{u} \in \mathcal{G} \cap \mathcal{A}_1$ implies u_1 and u_{-1} are constants. And this is possible only if V is constant.*

Proof. By Theorem 4.1, the Euler-Lagrange system (6) is reduced to the following two-component system:

$$\begin{cases} (\mu + \lambda) u_1 = \mathcal{L} u_1 + 2c_s u_1 (u_1^2 - u_{-1}^2) \\ (\mu - \lambda) u_{-1} = \mathcal{L} u_{-1} + 2c_s u_{-1} (u_{-1}^2 - u_1^2), \end{cases} \tag{16}$$

where $\mathcal{L} = -\Delta + V + 2c_n (u_1^2 + u_{-1}^2)$.

Recall that we assume $-N < M < N$, thus, for $j = 1, -1$, $u_j > 0$ on D. So $\mathbf{u} \in \mathcal{A}_1$ implies $u_{-1} = \kappa u_1$ for some constant $\kappa > 0$. Also note that $\kappa \neq 1$ since $M \neq 0$. The system (16) then gives the following two equations for u_1:

$$(\mu + \lambda)u_1 = -\Delta u_1 + Vu_1 + 2c_n(1 + \kappa^2)u_1^3 + 2c_s(1 - \kappa^2)u_1^3; \tag{17}$$

$$(\mu - \lambda)u_1 = -\Delta u_1 + Vu_1 + 2c_n(1 + \kappa^2)u_1^3 + 2c_s(\kappa^2 - 1)u_1^3. \tag{18}$$

Now (17) minus (18) gives $\lambda u_1 = 2c_s(1 - \kappa^2)u_1^3$. Since $u_1 > 0$ on D, we get

$$u_1 = \sqrt{\frac{\lambda}{2c_s(1 - \kappa^2)}}.$$

In particular u_1 and $u_{-1} = \kappa u_1$ are constants. Hence $\Delta u_1 = 0$, and then (17) plus (18) gives

$$\mu u_1 = Vu_1 + 2c_n(1 + \kappa^2)u_1^3,$$

from which we get

$$V = \mu - 2c_n(1 + \kappa^2)u_1^2 = \mu - \frac{c_n(1 + \kappa^2)}{c_s(1 - \kappa^2)}\lambda,$$

which is also a constant. □

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