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Long-Time Dynamics of the Schrödinger–Poisson–Slater System

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In this paper we analyze the asymptotic behaviour of solutions to the Schrödinger–Poisson–Slater (SPS) system in the frame of semiconductor modeling. Depending on the potential energy and on the physical constants associated with the model, the repulsive SPS system develops stationary or periodic solutions. These solutions preserve the $L^p(\mathbb{R}^3)$ norm or exhibit dispersion properties. In comparison with the Schrödinger–Poisson (SP) system, only the last kind of solutions appear.

KEY WORDS: Open quantum system; Schrödinger–Poisson system; dispersion; X^α-approach; asymptotic behaviour; stationary solutions.

1. INTRODUCTION

The aim of this paper is to analyze the asymptotic behaviour of solutions to the Schrödinger–Poisson–Slater (SPS) system.

The SPS system can be written in terms of the wave function $\psi: \mathbb{R}^3 \times [0, T[\to \mathbb{C}$ and the charge density $n(x, t) = |\psi(x, t)|^2$ as follows:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta_x \psi + V\psi - C_S n^{\frac{1}{3}} \psi, \qquad \lim_{|x| \to \infty} \psi(x, t) = 0, \tag{1}$$

$$\psi(x, t = 0) = \phi(x), \tag{2}$$

$$\Delta_x V = -\epsilon n, \qquad \lim_{|x| \to \infty} V(x, t) = 0, \tag{3}$$

where $\epsilon = 1$ (repulsive case) or $\epsilon = -1$ (attractive case) depending on the type of interaction considered. Here, $\hbar$ and m respectively hold for the

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Planck constant and the particle mass. Also, C_S stands for the Slater constant. The system coincides with the Schrödinger–Poisson (SP) system when the contribution of the last term (the Slater term) is not considered. As usual, Eqs. (1)–(3) are understood in a weak sense and (3) determines the self-consistent potential V originated by the charge of the particles. This potential can be equivalently written in integral form as

$$V(x,t)=\frac{\epsilon}{4\pi}\int_{\mathbb{R}^3}\frac{|\psi(x',t)|^2}{|x-x'|}\,dx'.$$

The physical constants ($\hbar, m$) that are usually involved in the formulation of the Schrödinger equation can be normalized to unity for the sake of simplicity. However, this normalization also modifies the Slater constant, whose value is relevant for the subsequent analysis.

The SPS system describes the evolution of an electron ensemble in a semiconductor crystal. The mixed-state SP system is commonly used to model semiconductor devices (see ref. 23). However, the repulsive effect of the Coulomb potential seems to be too strong when we compare the behaviour of the solutions to the SP system to simulations of superlattice structures (see refs. 25 and 27). These phenomena are also observed in the context of attractive Coulomb potential. Some different approximations have been studied to overcome this problem, obtaining appropriate adaptations of the Poisson potential. The Hartree–Fock model has been used to analyze a wide variety of phenomena in Quantum-Chemistry and Solid State Physics (see refs. 1, 16, and 22). The time-dependent Hartree–Fock equation has been analyzed in refs. 14 and 9. One of the most interesting corrections to the Poisson potential in the SP system is found by deriving nonlinear $|\psi|^\alpha$ terms from the Fock potential via various limits, in particular the low density limit,[(3)] which gives $\alpha=2/3$. This kind of $|\psi|^\alpha$ approximations to the Fock term is usually called the X^α-approach. Another motivation for this approximation in Quantum-Chemistry is the enormous quantity of calculations necessary to evaluate the Fock term, usually of order N^4, N being the number of particles. In this direction, the X^α approach to the Fock correction (Dirac, Slater,...) has been proved relevant in different contexts. These local approximations to nonlocal interaction terms give excellent results when studying stationary states, for example in Quantum Chemistry (see ref. 7 and refs. 17, 20, and 4 for some derivations and analysis of these systems). Then, the calculations are reduced from N^4 to N^3, even there might be some place for improvements. However, there is no rigorous foundation of the X^α-model in the time-dependent case. In this direction, following the classical ideas of the thermodynamical limit in Statistical Mechanics (see ref. 8) some recent advances are being done from the continuum and mean-field limit of the N-quantum-particle system by C. Bardos *et al.*, see ref. 2.

The aim of this work is to analyze the qualitative differences between the Schrödinger–Poisson–Slater ($\alpha = \frac{2}{3}$) evolution system and the Schrödinger–Poisson and Hartree–Fock systems. We are mainly interested in the X^{α} case studied in semiconductor theory, that is $\alpha = \frac{2}{3}$, which is derived from the Fock term by means of a low density limit, see ref. 3. This $|\psi|^{2/3}\,\psi$ correction is also known as the Dirac exchange term. Another interesting approach comes from the limit of heavy atoms, i.e., the high charge of nuclei limit; this leads to the Thomas–Fermi correction ($\alpha = 4/3$) of the kinetic energy, see refs. 17 and 18. In this paper we do not approximate the kinetic energy term (which is also called the von Weizsäcker correction). However, the Thomas–Fermi term can be alternatively seen as a correction of the Fock interaction, that always appears as a repulsive potential, see ref. 18. As we will point out later, these other X^{α}-approaches, useful in many scientific contexts, can be treated in our mathematical framework.

One important feature of the SPS system is that its associated potential energy can reach negative values depending on the constants of the system (mass, initial energy, or Slater constant). This fact implies some relevant properties of the SPS system in the repulsive case: (1) the minimum of the total energy operator is negative for some choices of the physical constants; (2) there are solutions (depending on the initial energy) that do not have dispersive character; (3) there are steady-state solutions, i.e., solutions with constant density; (4) there are solutions, even with positive energy, which preserve the L^p norm and do not decay with the time evolution. These properties show important qualitative differences between the SPS system and the SP and Hartree–Fock systems, see refs. 12, 6, 9, and 14. On the other hand, the X^{α}-Slater-model appears as an appropriate correction to the self-consistent Coulomb potential in semiconductor heterostructures modeling, in the sense that it covers different phenomenologies observed in this context. Some of our results hold true under the hypothesis of a relation between the value of the Slater constant, the mass and the energy of the system. However, the Slater constant is a characteristic of the component metals in the semiconductor device as it was pointed out in ref. 11 when interpreting the exchange-correlation potential of Kohn–Sham type. In this way, our study covers the whole range of variation for these constants, and the relation between these constants appears in a natural way and is not a restriction from a physical point of view. As we have commented before, the main differences with respect to the SP system occur in the repulsive case, where non dispersive effects, stationary and periodic solutions appear. However, the attractive case is also of interest in applications related to quantum gravity in the limit of very heavy particles (see, for example, ref. 24), thus we analyze both cases. We focus our study in the single-state case.

In ref. 3, the mixed-state case for the SPS system has been dealt with. In particular, the well-posedness and regularity of local-in-time and global solutions was analyzed, with L^2 or H^1 initial data. Also, the basic conservation laws and the minimal energy solutions in the attractive case were derived under a variational framework. A different approach for the single-state case can be seen in ref. 5.

Most of these results are valid for other X^α-approaches. However, motivated by the applications in semiconductor theory, we focus our efforts in the Slater approach to the Fock term. We will comment along the paper on some extensions of the results to other X^α-terms or some combination of them.

Let us summarize the main results and the techniques used in the paper in comparison with previous results. Section 2 is devoted to the minimization of the energy functional in the repulsive case. This allows us to deduce the existence of stationary solutions with negative energy as well as optimal bounds for the kinetic energy. To deal with this nonconvex minimization problem we can use different techniques introduced in refs. 17, 19, and 21. This problem was treated in ref. 3 (in the attractive case) by using symmetric decreasing rearrangement inequalities, but this tool seems to be fruitless in the repulsive case. Some minimization problems related to the repulsive case are studied in ref. 17 and in refs. 22 and 4 for small enough values of the mass upon using a perturbative argument. Alternatively, we propose here a scaling argument which provides effective bounds on the mass. In the third section we analize the long time behaviour of SPS solutions. The balance between the Coulombian potential and the Slater correction makes the usual arguments (based on the pseudo-conformal law) powerless. In our analysis we combine this property, or the equivalent dispersion equation, with the Galilean invariance in order to conclude some $L^p(\mathbb{R}^3)$ estimates. Also, from the dispersion equation (which relates the total energy to the momentum and position dispersions) it can be deduced that the solution is expansive in the sense that its second order moment increases with time. Finally, in Section 4 we analyze the asymptotic behaviour of the SPS solutions under attractive Coulomb forces. Actually, we prove the existence of stationary solutions in the case of negative energy.

2. MINIMUM OF THE ENERGY IN THE REPULSIVE CASE: STATIONARY SOLUTIONS, SOLUTIONS PRESERVING THE L^p NORM AND EVOLUTION OF THE KINETIC ENERGY

The Slater term introduces some qualitative differences in the behaviour of the solutions to the SPS system when compared to solutions to the

SP system. While the SP energy in the repulsive case is always positive, this can be negative when the Slater contribution is considered. The total energy operator associated with the solutions to the SPS system has the following form:

$$E[\psi] = \int_{\mathbb{R}^3} \left\{ \frac{|\nabla\psi(x,t)|^2}{2} + \int_{\mathbb{R}^3} \frac{\epsilon\, |\psi(x,t)|^2\, |\psi(x',t)|^2}{8\pi\, |x-x'|}\, dx' - \frac{3C_S}{4}\, |\psi(x,t)|^{\frac{8}{3}} \right\} dx. \tag{4}$$

E is an invariant of motion (i.e., E is preserved along the time evolution) provided that ψ is such that $E[\psi]$ is well-defined (see ref. 3). We refer to the first term in the right-hand side of (4) as the kinetic energy $E_{\mathrm{KIN}}(\psi)$, while the sum of the last two terms is the potential energy $E_{\mathrm{POT}}(\psi)$. In (4), the expression of the Coulombian potential has been identified as

$$\frac{1}{2}\int_{\mathbb{R}^3} V(x)\, n(x)\, dx = \frac{\epsilon}{2}\int_{\mathbb{R}^3} |\nabla V(x)|^2\, dx.$$

However, in the repulsive case $\epsilon = 1$, we can prove that the potential energy is always negative for some choice of the Slater constant in terms of the mass of the system. The following result corroborates this feature.

Lemma 2.1. If the $\mathrm{L}^2(\mathbb{R}^3)$ norm of the initial data ϕ associated with the SPS system verifies

$$\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)} \leqslant \left(\frac{3C_S}{2C}\right)^{\frac{3}{4}},$$

where C_S is the Slater constant and C is a positive constant determined by

$$\frac{1}{C} = \mathrm{Inf}\left\{ \frac{\|\psi(\cdot,t)\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}}{\|\nabla V(\psi)(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)}};\ \psi \in L^{\frac{8}{3}}(\mathbb{R}^3) \cap L^2(\mathbb{R}^3),\ \|\psi(\cdot,t)\|_{L^2} = 1 \right\},$$

then the potential energy of the solutions is negative along the time evolution.

Proof. This result is based on the following inequality, valid for all $\psi \in \mathrm{L}^2(\mathbb{R}^3) \cap L^{\frac{8}{3}}(\mathbb{R}^3)$:

$$\|\nabla V(\psi)(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \leqslant C\, \|\psi(\cdot,t)\|^{\frac{4}{3}}_{\mathrm{L}^2(\mathbb{R}^3)}\, \|\psi(\cdot,t)\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}. \tag{5}$$

This inequality is a direct consequence of Hölder and Hardy–Littlewood–Sobolev inequalities as well as of the interpolation inequalities for L^p spaces.

Applying (5) to solutions ψ of the SPS system and using that the L^2-norm of the initial data is preserved along the time evolution, we conclude the proof by writing

$$E_{\mathrm{POT}}(\psi)(t) \leqslant \left(\frac{C}{2} \|\psi(\cdot,t)\|_{L^2(\mathbb{R}^3)}^{\frac{4}{3}} - \frac{3}{4} C_{\mathrm{S}} \right) \|\psi(\cdot,t)\|_{L^{\frac{8}{3}}(\mathbb{R}^3)}^{\frac{8}{3}}. \quad \blacksquare$$

Remark. The inequality (5) as well as an upper bound for the sharp constant C were found by Lieb and Oxford in ref. 16. In our context, this bound takes the value $C = \frac{1.092}{2\pi} = 0.1737$.

Furthermore, since the potential energy associated with the initial data can be negative in the repulsive case we can find initial conditions for which the total energy is also negative, as proved in the following

Proposition 2.2. There exist initial data $\phi \in \mathrm{H}^1(\mathbb{R}^3)$ for which the total energy in the repulsive case is negative.

Proof. Let $\psi \in \mathrm{H}^1(\mathbb{R}^3)$ such that the associated potential energy is negative (this may happen by virtue of Lemma 2.1). Then, there is $\sigma > 0$ small enough such that the total energy of $\psi_\sigma(x) = \sigma^{\frac{3}{2}} \psi(\sigma x)$,

$$E[\psi_\sigma] = \sigma^2 E_{\mathrm{KIN}}(\psi) + \sigma E_{\mathrm{POT}}(\psi), \tag{6}$$

is nonpositive. Then, by choosing $\phi = \psi_\sigma$ as initial condition, the energy associated with this problem is nonpositive. $\blacksquare$

Remark. The same thing occurs when other X^α terms are considered. The total energy functional also reaches negative values when couplings of the Coulombian potential with power nonlinearities $|\psi|^\alpha \psi$, $\alpha \in (0, 4/3]$ are considered. Combinations of some of these terms could be also possible in their attractive or repulsive versions. However, some other kind of problems appear in the minimization argument, as we will mention in the next subsection.

Proposition 2.2 allows to remark some important differences between the asymptotic behaviour of solutions to our system and those to the SP system. For the repulsive SP system it was proved (see refs. 6 and 12) that the L^p norms of the solutions tend asymptotically in time to zero for $p \in]2, 6]$. However, when we analyze the evolution of solutions to the repulsive SPS system whose initial data has negative energy, we observe that the $L^{\frac{8}{3}}$ norm of the wave function ψ cannot go to zero as $t \to \infty$. This is because the total energy of the system is preserved and the Slater term is the only nonpositive contribution to the total energy.

One of the relevant points in the analysis of this problem is the existence of a global minimum of the energy functional in $H^1(\mathbb{R}^3)$ under the constraint $\|\psi\|_{L^2(\mathbb{R}^3)} = M$. This problem has no solution for the repulsive SP system because the infimum of the energy is always 0, which is not a minimum except for the case $M = 0$. In the following section we prove the existence of such a minimum for the SPS problem, for solutions with sufficiently small $L^2(\mathbb{R}^3)$ norm.

2.1. Minimum of Energy in the Repulsive Case

In this section we study the following minimization problem associated with the total energy of the repulsive SPS system

$$I_M = \inf\{E[\psi]; \psi \in H^1(\mathbb{R}^3), \|\psi\|_{L^2(\mathbb{R}^3)} = M\}, \tag{7}$$

where $M > 0$ and $E[\psi]$ is defined by (4). The main result of this section claims that this functional reaches a minimum value, which allows us to deduce two interesting consequences. The first one is the existence of stationary profiles, which are periodic-in-time solutions to the SPS system preserving the density. We also note that this kind of solutions does not exist for the repulsive SP system. The second consequence is the derivation of optimal bounds for the kinetic energy of solutions for which the total energy is well-defined.

Let us prove the results that ensure the existence of a minimum of (7). Firstly we observe that the energy operator is bounded from below in terms of the problem (7). From the Gagliardo–Nirenberg inequality we get

$$\frac{\|\psi\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}}{\gamma^{\frac{8}{3}}\,\|\psi\|^{\frac{5}{3}}_{L^2(\mathbb{R}^3)}} \leqslant \|\nabla\psi\|_{L^2(\mathbb{R}^3)}, \tag{8}$$

which holds for all $\psi(\cdot, t) \in H^1(\mathbb{R}^3)$. Using (8) and the fact that in this case the Coulombian potential term is nonnegative we obtain

$$E[\psi] \geqslant \left(\frac{\int_{\mathbb{R}^3} |\psi(x)|^{\frac{8}{3}}\,dx}{\gamma^{\frac{8}{3}} M^{\frac{5}{3}}}\right)^2 - \frac{3}{2} C_S \int_{\mathbb{R}^3} |\psi(x)|^{\frac{8}{3}}\,dx. \tag{9}$$

The right-hand side of (9) can be seen as a second order polynomial $ax^2 + bx$ in $\int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}}\,dx$, where

$$a = (\gamma^{\frac{8}{3}} M^{\frac{5}{3}})^{-2} \qquad \text{and} \qquad b = -\tfrac{3}{2} C_S.$$

Thus, we immediately conclude that the total energy is bounded from below. Furthermore, we can deduce the boundedness in $H^1(\mathbb{R}^3)$ of any minimizing sequence, which plays an important role in our argument to obtain the minimum of the functional.

The technical difficulties arising in this nonconvex minimization problem come from the invariance of the total energy functional by the non-compact group of translations. The possible loss of compactness due to that invariance has to be detected by the techniques used in the proofs. In this way, two methods are proposed in the previous literature to analize the class of problems (7): the concentration-compactness method[(21)] and the method of the nonzero weak convergence after translations.[(19)] In fact, we can prove that every minimizing sequence is *in essence* relatively compact provided that a certain sub-additivity property is strict. This condition implies that a minimizing sequence is *concentrated* in a bounded domain. Recently, this lack of compactness has been analyzed in ref. 10 for the Sobolev embedding. Since an important part of the intermediate steps are common to both (concentration-compactness and nonzero weak convergence after translations in Sobolev sapces) techniques, we will comment the application of them.

2.1.1. Concentration-Compactnes Argument

We can use the following formulation of the concentration-compactness principle adapted to our situation.

Proposition 2.3. For every $M > 0$, the following inequality

$$I_M \leqslant I_\alpha + I_{M-\alpha}, \qquad \forall \alpha \in (0, M), \tag{10}$$

holds. Furthermore, every minimizing sequence of (7) is relatively compact in $H^1(\mathbb{R}^3)$ (up to a translation) if and only if

$$I_M < I_\alpha + I_{M-\alpha}, \qquad \forall \alpha \in (0, M). \tag{11}$$

Proof. The proof is a consequence of Lemmas III.1 and I.1 in ref. 21. In order to make the paper self-consistent, we adapt these results to our notation. The general framework for minimization problems proposed by P. L. Lions allows us to establish the condition (10). Consider a minimizing sequence $\{u_n\}$ of (7). Since this sequence is bounded in $H^1(\mathbb{R}^3)$ with $\|u_n\|^2_{L^2(\mathbb{R}^3)} = M$, then there exists a subsequence $n_k \in \mathbb{N}$ for which either compactness or vanishing or dichotomy occurs (Lemma III.1, ref. 21). In order to prove compactness let us prove that vanishing and dichotomy cannot occur. The strict sub-additivity condition (11) prevents the subsequence from dichotomy. This property is stated as follows: there exists

$\alpha \in]0, M[$ such that for every $\varepsilon > 0$, there exist $k_0 \geqslant 1$ and u_k^1, u_k^2 bounded in $H^1(\mathbb{R}^3)$ satisfying

$$\begin{cases} \|u_{n_k} - (u_k^1 + u_k^2)\|_{L^p(\mathbb{R}^3)} \leqslant \delta_p(\epsilon) \to 0, \qquad \epsilon \to 0^+, \quad 2 \leqslant p < 6; \\ \left|\int_{\mathbb{R}^3} |u_k^1|^2\, dx - \alpha\right| \leqslant \varepsilon, \qquad \left|\int_{\mathbb{R}^3} |u_k^2|^2\, dx - (M-\alpha)\right| \leqslant \varepsilon; \\ \operatorname{dist}(\operatorname{Supp} u_k^1, \operatorname{Supp} u_k^2) \to \infty, \qquad k \to \infty; \\ \liminf_k \int_{\mathbb{R}^3} \{|\nabla u_{n_k}|^2 - |\nabla u_k^1|^2 - |\nabla u_k^2|^2\}\, dx \geqslant 0; \end{cases}$$

for $k \geqslant k_0$. Indeed, if dichotomy occurs we easily deduce that

$$I_M \geqslant I_\alpha + I_{M-\alpha},$$

which yields a contradiction. On the other hand, if strict sub-additivity does not occur, then a minimizing sequence can be constructed without convergent subsequences (see ref. 21 for details). Vanishing occurs when

$$\lim_{k\to\infty} \sup_{y \in \mathbb{R}^3} \int_{y+B_R} |u_{n_k}(x)|^2\, dx = 0, \qquad \forall R < \infty, \quad B_R = \{x \in \mathbb{R}^3, |x| < R\}.$$

It can be proved that the subsequence does not vanish as follows from the fact that $I_M < 0$ and from the following result (Lemma I.1, ref. 21 with $q = 2$, $p = 2$, and $\alpha = 8/3$):

Lemma 2.4. Let $1 < p \leqslant \infty$ and $1 \leqslant q < \infty$ with $q \neq \frac{3p}{3-p}$ if $p < 3$. Assume that u_n is bounded in $L^q(\mathbb{R}^3)$, ∇u_n is bounded in $L^p(\mathbb{R}^3)$ and

$$\sup_{y \in \mathbb{R}^3} \int_{y+B_R} |u_n|^q\, dx \underset{n}{\longrightarrow} 0 \qquad \text{for some} \quad R > 0.$$

Then, $u_n \underset{n}{\longrightarrow} 0$ in $L^\alpha(\mathbb{R}^3)$ for $\alpha \in [q, \frac{3p}{3-p}]$.

Hence, we have proved that any minimizing sequence satisfies the following compactness criterium: there exists $y_k \in \mathbb{R}^3$ such that $|u_{n_k}(\cdot + y_k)|^2$ is tight

$$\forall \varepsilon > 0, \qquad \exists R < \infty, \qquad \int_{y_k+B_R} |u_{n_k}(x)|^2 \geqslant M - \varepsilon.$$

Setting $\tilde{u}_n = u_n(\cdot + y_n)$, we can assume (up to a subsequence) that $\tilde{u}_n \to \tilde{u}$ weakly in $\mathrm{H}^1(\mathbb{R}^3)$ and the compactness property implies

$$\int_{B_R} |\tilde{u}|^2\, dx \geqslant M - \varepsilon.$$

Thus, $\tilde{u}_n$ converges strongly in $\mathrm{L}^2(\mathbb{R}^3)$ to $\tilde{u}$. By using the Gagliardo–Nirenberg inequality, $\tilde{u}_n$ converges strongly to $\tilde{u}$ in $\mathrm{L}^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$. This fact allows to assure that $\tilde{u}$ is a minimum of the problem I_M as consequence of the weak lower semi-continuity of the $\mathrm{H}^1(\mathbb{R}^3)$ norm and the convergence $E_{\mathrm{POT}}(\tilde{u}_n) \to E_{\mathrm{POT}}(\tilde{u})$. Thus, *a posteriori* we deduce

$$\int_{\mathbb{R}^3} |\nabla \tilde{u}_n|^2\, dx \xrightarrow[n]{} \int_{\mathbb{R}^3} |\nabla \tilde{u}|^2\, dx,$$

showing the compactness in $\mathrm{H}^1(\mathbb{R}^3)$. ∎

To obtain the relative compactness of any minizing sequence (up to translations) has been used the concentration-compactness argument that can be equivalently replaced by the arguments based on nonzero weak convergence after translations.[19] The point which is common to both techniques is that hypothesis (11) is required.

2.1.2. Nonzero Weak Convergence after Translations

In this approach, we apply the next two results to any minimizing sequence $\{u_n\}_{n\in\mathbb{N}}$ of (7) to guarantee the existence of a nonzero weak convergent subsequence in $\mathrm{H}^1(\mathbb{R}^3)$ up to translations (see ref. 19, Theorem 8.10, and exercise 2.22, for more details):

Lemma 2.5 (Exercise 2.22, ref. 19). Suppose that $1 \leqslant p < q < r \leqslant \infty$ and that u is a function in $\mathrm{L}^p(\Omega) \cap \mathrm{L}^r(\Omega)$ with $\|u\|_{\mathrm{L}^p(\Omega)} \leqslant C_p < \infty$, $\|u\|_{\mathrm{L}^r(\Omega)} \leqslant C_r < \infty$, and $\|u\|_{\mathrm{L}^q(\Omega)} \geqslant C_q > 0$. Then, there are constants $\epsilon > 0$ and $M > 0$, depending only on p, q, r, C_p, C_q, C_r, such that $Meas(\{x\colon |u(x)| > \epsilon\}) > M$.

Theorem 2.6 (Theorem 8.10, ref. 19). Let $1 < p < \infty$ and let $\{u_n\}_{n\in\mathbb{N}}$ be a bounded sequence of functions in $\mathrm{H}^1(\mathbb{R}^3)$. Suposse that for some $\epsilon > 0$ the set $E_n := \{x\colon |u_n(x)| > \epsilon\}$ satisfies $Meas(E_n) > \delta > 0$ for some δ and all $n \in \mathbb{N}$. Then, there is a sequence of vectors $y_n \in \mathbb{R}^3$ such that the translated sequence $\tilde{u}_n(x) := u(x + y_n)$ has a subsequence that converges weakly in $\mathrm{H}^1(\mathbb{R}^3)$ to a nonzero function.

Any function u_n verifies the hypothesis of Lemma 2.5 with $p = 2$, $q = 8/3$, $p = 6$, $C_p = M$, and $C_q = (-4I_M/3C_S)^{\frac{8}{3}}$, C_r being a constant which comes from the boundedness of $\{u_n\}_{n\in\mathbb{N}}$ in $\mathrm{H}^1(\mathbb{R}^3)$. Then, the whole sequence satisfies the hypotheses of Theorem 2.6. As consequence, there exist vectors y_n such that a subsequence of u_n verifies

$$\tilde{u}_n := u_n(\cdot + y_j) \to \tilde{u} \quad \text{weakly in } \mathrm{H}^1(\mathbb{R}^3), \qquad \|\tilde{u}\|_{\mathrm{H}^1(\mathbb{R}^3)} > 0. \tag{12}$$

In order to deduce that $\tilde{u}$ is a minimizer of (7) we have to prove that

$$E_{\mathrm{POT}}(\tilde{u}) \leqslant \liminf E_{\mathrm{POT}}(\tilde{u}_n).$$

To this aim, it is enough to observe that no charge *escapes* to infinity, i.e., $\|\tilde{u}\|_{\mathrm{L}^2(\mathbb{R}^3)} = M$, because this would imply the convergence $\tilde{u}_n \to \tilde{u}$ in $\mathrm{L}^2(\mathbb{R}^3)$ and $E_{\mathrm{POT}}(\tilde{u}_n) \to E_{\mathrm{POT}}(\tilde{u})$. The inequality (11) plays a crucial role at this point. If $\|\tilde{u}\|_{\mathrm{L}^2(\mathbb{R}^3)} = \alpha < M$, then it can be proved that $\tilde{u}_n$ is under the dichotomy hypothesis. Indeed, there exists $R > 0$ such that $\int_{B_R} |\tilde{u}|^2\, dx = \alpha - \epsilon/2$, for $\epsilon > 0$. On the other hand, let R_n be such that $\int_{B_{R_n}} |\tilde{u}_n|^2\, dx = \alpha + \epsilon/2$. The sequence $\{R_n\}_{n\in\mathbb{N}} \to \infty$ as $n \to \infty$ (otherwise, this would contradict (12)). We define $\tilde{u}_n^1 := \tilde{u}_n \chi_{B_R}$ and $\tilde{u}_n^2 := \tilde{u}_n \chi_{\mathbb{R}^3 - B_{R_n}}$, where $n \in \mathbb{N}$ and χ_Ω denotes the characteristic function of the set Ω. Then, we have that $\{\tilde{u}_n\}$ verifies

$$\begin{cases} \|\tilde{u}_n - (\tilde{u}_n^1 + \tilde{u}_n^2)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leqslant \delta_p(\epsilon) \to 0, \qquad \epsilon \to 0^+, \quad 2 \leqslant p < 6; \\ \left| \int_{\mathbb{R}^3} |\tilde{u}_n^1|^2\, dx - \alpha \right| \leqslant \epsilon, \qquad \left| \int_{\mathbb{R}^3} |\tilde{u}_n^2|^2\, dx - (M - \alpha) \right| \leqslant \epsilon; \\ \mathrm{dist}(\mathrm{Supp}\, \tilde{u}_n^1, \mathrm{Supp}\, \tilde{u}_n^2) = R_n - R \to \infty, \qquad n \to \infty; \\ \liminf_k \int_{\mathbb{R}^3} \{|\nabla \tilde{u}_n|^2 - |\nabla \tilde{u}_n^1|^2 - |\nabla \tilde{u}_n^2|^2\}\, dx \geqslant 0; \end{cases}$$

for $n \geqslant n_0$. The incompatibility between dichotomy and (11) allows to conclude that $\|\tilde{u}\|_{\mathrm{L}^2(\mathbb{R}^3)} = M$ as well as the minimizing charater of $\tilde{u}$. This concludes the proof with the technique of nonzero weak convergence after translations in Sobolev spaces.

Before deriving the inequality (11) in the SPS context, let us introduce some notations. Let a, b, c be positive constants and consider the operators $T_{\mathrm{KIN}}, T_{\mathrm{POT}}, T, K\colon\ \mathrm{H}^1(\mathbb{R}^3) \longrightarrow \mathbb{R}$ defined by

$$T_{\mathrm{KIN}}(\psi) = a \int_{\mathbb{R}^3} |\nabla \psi(x)|^2\, dx,$$

$$T_{\mathrm{POT}}(\psi) = \int_{\mathbb{R}^3} \left\{ b \int_{\mathbb{R}^3} \frac{|\psi(x)|^2\, |\psi(x')|^2}{|x - x'|}\, dx' - c\, |\psi(x)|^{\frac{8}{3}} \right\} dx,$$

$$T(\psi) = T_{\mathrm{KIN}}(\psi) + T_{\mathrm{POT}}(\psi), \qquad K(\psi) = -\frac{1}{4} \frac{(T_{\mathrm{POT}}(\psi))^2}{T_{\mathrm{KIN}}(\psi)}.$$

Then, we have the following

Lemma 2.7. The minimization problems associated with the operators T and K over the set

$$\mathscr{B}_M = \{\psi \in \mathrm{H}^1(\mathbb{R}^3);\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M,\ T_{\mathrm{POT}}(\psi) < 0\}$$

are equivalent in the following sense

$$T_M \equiv \inf\{T[\psi];\ \psi \in \mathscr{B}_M\} = \inf\{K[\psi];\ \psi \in \mathscr{B}_M\} \equiv K_M.$$

In addition, if ψ is a function in which T achieves its minimum, then it is also the minimum for the functional K. On the other hand, if ψ is a function in which K achieves its minimum, then the function ψ^σ is a minimum for T, where $\psi^\sigma(x) = \sigma^{\frac{2}{3}}\psi(\sigma x)$ and $\sigma = \frac{-T_{\mathrm{POT}}(\psi)}{2T_{\mathrm{KIN}}(\psi)}$.

Proof. We first remark that the scaling $\psi^\sigma(x) = \sigma^{\frac{3}{2}}\psi(\sigma x)$, $\sigma > 0$, preserves the properties of $\mathscr{B}_M$. Then, the result can be easily deduced by optimizing for every $\psi \in \mathscr{B}_M$ the value of the parameter σ for which the total energy reaches the minimum over the uniparametric family of functions $\{\psi^\sigma;\ \sigma \in \mathbb{R}^+\}$. ∎

As a particular case, we obtain a minimization problem equivalent to (7). Denoting $\mathscr{A}_M = \{\psi \in \mathrm{H}^1(\mathbb{R}^3);\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M,\ E_{\mathrm{POT}}[\psi] < 0\}$, we have

$$I_M = \inf\{E[\psi];\ \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\} = \inf\{E[\psi];\ \psi \in \mathscr{A}_M\},$$

which shows that our problem is equivalent to

$$\inf\left\{-\frac{1}{4}\frac{(E_{\mathrm{POT}}(\psi))^2}{E_{\mathrm{KIN}}(\psi)};\ \psi \in \mathscr{A}_M\right\}. \tag{13}$$

Also, note that the set $\mathscr{A}_M$ is nonempty for any value of M, see refs. 22 and 4.

Furthermore we have $-E_{\mathrm{POT}}(\psi_M) = 2E_{\mathrm{KIN}}(\psi_M)$, where ψ_M denotes the minimizer of I_M. Consequently,

$$E(\psi_M) = \tfrac{1}{2}E_{\mathrm{POT}}(\psi_M) = -E_{\mathrm{KIN}}(\psi_M). \tag{14}$$

Using Lemma 2.7 we can prove the following result, which provides the strict sub-additivity property (11).

Proposition 2.8. For all $C_{\mathrm{S}} > 0$ and $M > 0$ such that

$$M < \left(\frac{7C_{\mathrm{S}}}{10C}\right)^{\frac{3}{4}}, \tag{15}$$

the sub-additivity condition (11) holds. Here, C_{S} denotes the Slater constant and C is the sharp constant in (5).

Proof. Assume that M satisfies (15). Using the scaling

$$\psi(x) \longrightarrow M^4 \psi(M^2 x),$$

the set $\mathcal{A}_M$ can be seen, for each $M \in \mathbb{R}^+$, as a transformation of the set

$$\mathcal{B}'_M := \{\psi \in \mathrm{H}^1(\mathbb{R}^3);\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1,\ E^M_{\mathrm{POT}}(\psi) < 0\},$$

where

$$E^M_{\mathrm{POT}}(\psi) = \frac{M^6}{8\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\psi(x)|^2\,|\psi(y)|^2}{|x-y|}\,dx\,dy - \frac{3C_{\mathrm{S}} M^{\frac{14}{3}}}{4} \int_{\mathbb{R}^3} |\psi(x)|^{\frac{8}{3}}\,dx.$$

In the same way, (7) can be rewritten as

$$I_M = \inf\{E^M_{\mathrm{KIN}}(\psi) + E^M_{\mathrm{POT}}(\psi);\ \psi \in \mathcal{B}'_M\},$$

where $E^M_{\mathrm{KIN}}(\psi) = \frac{M^6}{2} \int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx$. Since $E^M_{\mathrm{POT}}(\psi) < 0$ by (15) and the proof of Lemma 2.1, we can take $\mathcal{B}'_M = \{\psi \in \mathrm{H}^1(\mathbb{R}^3);\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1\}$. Under this assumption, our minimization problem reads

$$I_M = M^{\frac{14}{3}-p} \inf\left\{ \frac{M^{\frac{4}{3}+p}}{2} \int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx + \frac{M^{\frac{4}{3}+p}}{8\pi} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\psi(x)|^2\,|\psi(y)|^2}{|x-y|}\,dx\,dy \right.$$
$$\left. - \frac{3C_{\mathrm{S}} M^p}{4} \int_{\mathbb{R}^3} |\psi(x)|^{\frac{8}{3}}\,dx;\ \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1 \right\},$$

where p is a positive parameter to be precised. Then, we can apply Lemma 2.7 to show that this problem is equivalent to

$$I_M = M^{\frac{14}{3}-p} \inf\left\{ -\frac{\left(M^{\frac{2}{3}+\frac{p}{2}} \int_{\mathbb{R}^3} |\nabla V(\psi)|^2\,dx\,dy - \frac{3C_{\mathrm{S}}}{2} M^{\frac{p}{2}-\frac{2}{3}} \int_{\mathbb{R}^3} |\psi(x)|^{\frac{8}{3}}\,dx\right)^2}{8 \int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx}; \right.$$
$$\left. \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1 \right\} \stackrel{\mathrm{def}}{=} M^{\frac{14}{3}-p} I^M_1.$$

Now (11) can be written as

$$M^{\frac{14}{3}-p} I^M_1 < \alpha^{\frac{14}{3}-p} I^{\alpha}_1 + (M-\alpha)^{\frac{14}{3}-p} I^{M-\alpha}_1, \qquad \forall \alpha \in (0, M). \tag{16}$$

This inequality is based on the bound

$$M^k > \alpha^k + (M-\alpha)^k, \qquad \forall \alpha \in (0, M), \quad M \in \mathbb{R}^+, \quad \forall k > 1.$$

We easily deduce

$$M^{\frac{14}{3}-p} I_1^M < \alpha^{\frac{14}{3}-p} I_1^M + (M-\alpha)^{\frac{14}{3}-p} I_1^M, \qquad \forall \alpha \in (0, M),$$

for some $p \in (\frac{4}{3}, \frac{11}{3})$. To get (16) it is enough to show that for all $\eta \in (0, M)$, $I_1^M \leqslant I_1^\eta$ holds. This is true according to the nonincreasing character of the function

$$f_\psi : \eta \longrightarrow -\frac{1}{8} \frac{(\eta^{\frac{2}{3}+\frac{p}{2}} \int_{\mathbb{R}^3} |\nabla V(\psi)|^2 \, dx - \frac{3C_S}{2} \eta^{\frac{p}{2}-\frac{2}{3}} \int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}} \, dx)^2}{\int_{\mathbb{R}^3} |\nabla \psi|^2 \, dx},$$

for $\eta \in (0, M)$ and $p \in (\frac{4}{3}, \frac{11}{3})$, independently of ψ. Indeed, given M there exists $p \in (\frac{4}{3}, \frac{11}{3})$ such that

$$\frac{df_\psi}{d\eta} = -\frac{1}{4} \frac{1}{\int_{\mathbb{R}^3} |\nabla \psi|^2 \, dx} \left(\eta^{\frac{2}{3}+\frac{p}{2}} \int_{\mathbb{R}^3} |\nabla V(\psi)|^2 \, dx - \frac{3C_S}{2} \eta^{\frac{p}{2}-\frac{2}{3}} \int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}} \, dx \right)$$

$$\times \left(\left(\frac{2}{3} + \frac{p}{2} \right) \eta^{\frac{p}{2}-\frac{1}{3}} \int_{\mathbb{R}^3} |\nabla V(\psi)|^2 \, dx \, dy - \left(\frac{p}{2} - \frac{2}{3} \right) \frac{3C_S}{2} \eta^{\frac{p}{2}-\frac{5}{3}} \int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}} \, dx \right)$$

is nonpositive for every $\psi \in \mathscr{B}_M$, where we have used (5). The optimal bound is obtained as p approaches $\frac{11}{3}$. Finally, this allows to establish the inequality $I_1^M \leqslant I_1^\eta$, which concludes the proof. ▮

Remark. It is not clear to the authors if the constant in (15) is or not optimal. Some idea about its optimality could open the discussion on the nonexistence of minimizers when (11) in Proposition 2.3 is violated.

Remark. Note that the Thomas–Fermi correction usually appears with positive sign (see ref. 18), which can be seen as a repulsive contribution to the potential. Then, the addition of this kind of correction simplifies the minimizing argument because combining the repulsive Thomas–Fermi with the attractive Slater correction allows to convexify the functional, see ref. 17.

Now, a simple application of Propositions 2.3 and 2.8 yields the existence of a minimum, since every minimizing sequence is bounded in $H^1(\mathbb{R}^3)$ and relatively compact (up to a translation). Furthermore, by standard arguments (see ref. 15) the regularity of the minimum can be deduced.

Theorem 2.9. Under the hypothesis of Proposition 2.8, there exists a minimizer $\psi_M \in C^\infty(\mathbb{R}^3)$ of (7) which satisfies the following Euler–Lagrange equation associated with the total energy functional $E[\psi]$:

$$-\frac{1}{2}\Delta\psi_M(x)+\frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{|\psi_M(x')|^2\,\psi_M(x)}{|x-x'|}\,dx' - C_S\,|\psi_M|^{\frac{2}{3}}\,\psi_M(x)=\beta\psi_M(x) \quad (17)$$

in a distributional sense, for some $\beta<0$.

The following paragraph is devoted to show some consequences of this result.

2.1.3. Stationary Solutions and Solutions Preserving the L^p Norm in the Repulsive Case with Negative Energy

From Theorem 2.9 we can deduce the existence of standing waves $\psi(x,t)=e^{-i\beta t}\psi(x)$ as solutions of the SPS system in the repulsive case. Actually, these are time-periodic solutions which preserve the density. For this kind of solutions, the repulsive SPS system is reduced to the time-independent Schrödinger equation

$$\beta\psi=-\tfrac{1}{2}\Delta\psi+V\psi-C_S n^{\frac{1}{3}}\psi, \qquad \lim_{|x|\to\infty}\psi=0, \tag{18}$$

coupled to the Poisson equation

$$\Delta V=|\psi|^2, \qquad \lim_{|x|\to\infty}V=0. \tag{19}$$

The system (18) and (19) can be written as an Euler–Lagrange equation associated with (7) (cf. (17)). Then, Theorem 2.9 implies the existence of solutions ψ_M. Since these functions minimize the total energy operator, (14) holds.

Let us also note that this kind of solutions do not exist for the SP system in the repulsive case, where every solution is dispersive.

Let us now introduce some other solutions which preserve the L^p norm.

Proposition 2.10. There exist solutions of the SPS system with negative potential energy and constant L^p norm along the time evolution.

Proof. The proof is based on the Galilean invariance of the system, see ref. 3. In fact, this property guarantees that if $\psi(x,t)$ is a solution to the SPS system with initial data ψ_0, then the solution corresponding to initial data $\psi_N(x,0)=e^{iNx}\psi_0(x)$, with $N\in\mathbb{R}^3$, is $\psi_N(x,t)=e^{iNx-itN^2}\psi(x-2tN,t)$.

Now, using the minimal energy solution we can construct the solution $e^{-i\beta t}e^{iNx-it\frac{N^2}{2}}\psi_M(x-tN)$, which has initial data $e^{iNx}\psi_M(x)$. This solution preserves the L^p norm, has negative potential energy and its total energy is

$$E(e^{-i\beta t}e^{iNx-it\frac{N^2}{2}}\psi_M(x-tN))=\tfrac{1}{2}N^2\|\psi_M\|_{L^2(\mathbb{R}^3)}+I_M,$$

which obviously exceeds the minimal energy. A similar idea has been used in ref. 13. ▮

2.1.4. Optimal Kinetic Energy Bounds

Minimizing the total energy functional implies, by Lemma 2.7, the minimization of the associated functional

$$T(\psi)=-\frac{1}{4}\frac{(E_{\text{POT}}(\psi))^2}{E_{\text{KIN}}(\psi)}.$$

In the next result we use this fact to deduce optimal bounds for the kinetic energy of a solution, depending on the initial total energy and the minimum of the energy functional.

Proposition 2.11. The kinetic energy associated with a solution of the repulsive SPS system in $H^1(\mathbb{R}^3)$, E_{KIN}, ranges between the optimal values

$$E^{\pm}_{\text{KIN}}=-2I_M\left(1-\frac{E_0}{2I_M}\pm\sqrt{1-\frac{E_0}{I_M}}\right), \tag{20}$$

where E_0 is the initial energy and I_M is the infimum of the total energy over the set $\{\psi\in H^1(\mathbb{R}^3);\ \|\psi\|_{L^2(\mathbb{R}^3)}=M\}$. Here, M is assumed to satisfy (15).

Proof. As before, this is a direct consequence of the equivalence between the energy minimization problem and (13). Since ψ_M minimizes (7), we have

$$-\frac{1}{4}\frac{(E_{\text{POT}}(\psi))^2}{E_{\text{KIN}}(\psi)}\geqslant-\frac{1}{4}\frac{(E_{\text{POT}}(\psi_M))^2}{E_{\text{KIN}}(\psi_M)}=-\frac{1}{4}\frac{4\,I_M^2}{-I_M}=I_M,$$

for all $\psi\in H^1(\mathbb{R}^3)$ such that $\|\psi\|_{L^2(\mathbb{R}^3)}=M$. Then, given $\psi(\cdot,t)\in H^1(\mathbb{R}^3)$ a solution of the SPS system we find

$$E_{\text{POT}}(\psi)\geqslant-2\sqrt{-I_M}\sqrt{E_{\text{KIN}}(\psi)},\qquad \forall t\geqslant 0.$$

This yields a relation between the kinetic and the total energy:

$$E_0(\psi) \geqslant -2\sqrt{-I_M}\,\sqrt{E_{\mathrm{KIN}}(\psi)} + E_{\mathrm{KIN}}(\psi) \qquad \forall t \geqslant 0,$$

or, using that the potential energy is negative,

$$E_{\mathrm{KIN}}^2 + (4I_M - 2E_0)\, E_{\mathrm{KIN}} + E_0^2 \leqslant 0.$$

This concludes the proof. ∎

3. ASYMPTOTIC BEHAVIOUR IN THE REPULSIVE CASE

In this section we study the time evolution of solutions to the SPS system. The standard arguments used to obtain various bounds on the $L^p(\mathbb{R}^3)$ norms of solutions to nonlinear Schrödinger equations are fruitless in our case. This is due to the fact that the sign of the potential energy depends on the balance between the Coulombian potential and the Slater correction. Then, we have to combine these arguments with some other techniques to find the $L^p(\mathbb{R}^3)$ bounds.

By using similar arguments to those of ref. 26 we can derive an equation which models the dispersion of solutions to the SPS system. Let us define

$$(\Delta x)^2 \stackrel{\mathrm{def}}{=} \langle x^2\rangle(t) - \langle x\rangle^2(t) \qquad \text{and} \qquad (\Delta p)^2 \stackrel{\mathrm{def}}{=} \langle p^2\rangle(t) - \langle p\rangle^2(t),$$

where $\langle x\rangle(t)$ denotes the expected value for the position operator

$$\langle x\rangle(t) = \int_{\mathbb{R}^3} \psi^*(x,t)\, x\psi(x,t)\, dx,$$

while $\langle p\rangle(t)$ is the expected value for the linear momentum operator

$$\langle p\rangle(t) = \frac{1}{i}\int_{\mathbb{R}^3} \psi^*(x,t)\, \nabla\psi(x,t)\, dx, \tag{21}$$

which is preserved along the time evolution (see ref. 3). In terms of these operators we can prove the following result.

Theorem 3.1. The position and momentum dispersions for a solution $\psi(x,t)$ of the SPS system with initial data in $\Sigma = \{u \in H^2(\mathbb{R}^3);\ xu \in L^2(\mathbb{R}^3)\}$ satisfy the following equation

$$\frac{d^2}{dt^2}(\Delta x)^2(t) = 2\left(E(t) - \frac{1}{2}\langle p\rangle^2(t)\right) + (\Delta p)^2(t),$$

or equivalently

$$\frac{d^2}{dt^2}\langle x^2\rangle = 2\left(\frac{1}{2}\langle p^2\rangle + E(t)\right), \tag{22}$$

where $E(t)$ denotes the total energy.

By simple computations starting from the dispersion equation (22) we can deduce the pseudo-conformal law verified by a SPS solution $\psi(t, x)$:

$$\frac{d}{dt}\left(\|(x+it\nabla)\,\psi\|^2_{L^2(\mathbb{R}^3)} + t^2\int_{\mathbb{R}^3} Vn\,dx - \frac{3}{2}C_S t^2\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\,dx\right)$$
$$= t\int_{\mathbb{R}^3} Vn\,dx - \frac{3}{2}C_S t\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\,dx. \tag{23}$$

This shows an alternative derivation for the pseudo-conformal law widely studied in the literature (refs. 5 and 12).

Equation (22) allows to deduce (for positive energies) some important consequences about the long time behaviour of the solutions. The first one is that the solutions tend to expand unboundedly when the energy is positive. The second consequence is a decay bound for the potential energy.

Proposition 3.2. Let $\phi \in \Sigma$ the initial data of the SPS system such that $E(\phi) > 0$. Then, the system expands unboundedly for large times and the position dispersion $\langle x^2\rangle(t)$ grows like $O(t^2)$.

Proof. To deduce this result we consider again the dispersion equation (22), rewritten as

$$\frac{1}{2}\frac{d^2}{dt^2}\langle x^2\rangle = E_{\mathrm{KIN}} + E(t) = 2E(t) - E_{\mathrm{POT}}. \tag{24}$$

Since $\|\phi\|_{L^2} = M$ and $E(\phi) \equiv E$ are time invariant, we can bound the right-hand side of (24) by using (20) and obtain

$$E + E^-_{\mathrm{KIN}} \leqslant \frac{1}{2}\frac{d^2}{dt^2}\langle x^2\rangle \leqslant E + E^+_{\mathrm{KIN}}.$$

By using the lower bound of the Slater potential, we also find

$$E < \frac{1}{2}\frac{d^2}{dt^2}\langle x^2\rangle \leqslant 2E + C_{(E,M)}.$$

If E is positive, then the upper and lower bounds are also positive. This allows to deduce the result by integrating twice in time. ▮

As an immediate consequence we can deduce lower bounds for the L^p norm of the solutions. These lower bounds are either positive constants or coincide with the usual decay rates of the free Schrödinger equation, depending on a relation between the total energy, the mass and the linear momentum (21). For simplicity we shall denote $M[\psi] \equiv \langle p \rangle(0) = \frac{1}{i} \int_{\mathbb{R}^3} \psi^*(x)\, \nabla\psi(x)$.

Corollary 3.3. Let ψ be a SPS solution with initial data $\phi \in \Sigma$ such that

$$E[\phi] < \frac{1}{2} \frac{|M[\phi]|^2}{\|\phi\|_{L^2(\mathbb{R}^3)}}. \tag{25}$$

Then, there exist positive constants C, C', and C'' depending on $\|\phi\|_{L^2(\mathbb{R}^3)}$, $E[\phi]$, $|M[\phi]|^2$ and p such that

$$\|\psi(t)\|_{L^p(\mathbb{R}^3)} \geqslant C, \quad E_{\mathrm{POT}}[\psi] \leqslant -C', \qquad \forall t \geqslant 0, \quad p \in [\tfrac{8}{3}, 6]. \tag{26}$$

In the case

$$E[\phi] \geqslant \frac{1}{2} \frac{|M[\phi]|^2}{\|\phi\|_{L^2(\mathbb{R}^3)}}, \tag{27}$$

the following lower bound

$$\|\psi(\cdot, t)\|_{L^p(\mathbb{R}^3)} \geqslant \frac{C''}{t^{\frac{3p-6}{2p}}}, \qquad \forall t > \xi > 0, \quad p \in [2, 6], \tag{28}$$

holds.

Proof. To show the relevance of (25) and (27) we shall use again the Galilean invariance of the system. The solutions ψ_N associated with an initial condition $\phi_N = e^{iNx}\phi_0(x)$ have the same $L^p(\mathbb{R}^3)$ norm and the same potential energy for every N and time t, while the total energy is

$$E[\phi_N] = \tfrac{1}{2} N^2 \|\phi_N\|_{L^2(\mathbb{R}^3)} + N M[\phi] + E[\phi_0].$$

It is a simple matter to observe that for every ϕ_0 the Galilean invariance gives a parametric family of initial data ϕ_N for which the time evolution of the $L^p(\mathbb{R}^3)$ norm and of the potential energy are the same. The analysis of a particular member of the family of Galilean transformations allows to deduce the behaviour of the $L^p(\mathbb{R}^3)$ norm and of the potential energy for the whole family.

By a simple optimization argument one can easily check that (25) implies the existence of initial data with negative energy in the family, while the energy of the initial data is nonnegative if (27) holds.

Under hypothesis (27), the initial data ϕ can be assumed to have positive energy (if not, ϕ can be replaced by $\phi_{N'}$ belonging to the class of Galilean transforms of ϕ with positive energy). We have

$$\begin{aligned}\|\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} &= \int_{|x|\leqslant R} |\psi(x,t)|^2\,dx + \int_{|x|\geqslant R} |\psi(x,t)|^2\,dx,\\ &\leqslant CR^{\frac{3p-6}{p}} \|\psi(x,t)\|^2_{L^p(\mathbb{R}^3)} + \frac{1}{R^2}\langle x^2\rangle.\end{aligned}$$

By optimizing over R we obtain

$$\|\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} \leqslant C(\|\psi(\cdot,t)\|_{L^p(\mathbb{R}^3)})^{\frac{4p}{5p-6}} \langle x^2\rangle^{\frac{3p-6}{5p-6}}.$$

This concludes (28) by using Proposition 3.2 and the positivity of the total energy.

On the other hand, if ϕ fulfills (25), then we can choose a Galilean translation $\phi_{N'}$ whose total energy is negative. In this case, we find

$$-\|\psi_{N'}(t)\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)} < E[\phi_{N'}] < 0, \qquad \forall t \geqslant 0.$$

We conclude (28) by using the Hölder inequality, mass preservation and the invariance of the L^p norm of the solutions under Galilean translations. ▮

The next result provides a rate-of-decay estimate for the potential energy. However, the potential energy may be negative as shown before. For instance, from (5) we know that the potential energy is always nonpositive in the repulsive case.

Proposition 3.4. Let $\phi \in \Sigma$ the initial data of the SPS system. Then, the potential energy associated with the solution $\psi(x,t)$ satisfies the inequality

$$E_{\mathrm{POT}}(\psi)(t) \leqslant \frac{C_\xi}{t}, \qquad \forall t \geqslant \xi > 0, \tag{29}$$

where C_ξ is a positive constant depending on ξ.

Proof. Integrating the pseudo-conformal law from ξ to t we find

$$\|(x+it\nabla)\,\psi(\cdot\,,t)\|^2_{L^2(\mathbb{R}^3)}+t^2\int_{\mathbb{R}^3}|\nabla V(x,t)|^2\,dx-\frac{3}{2}\,C_S t^2\int_{\mathbb{R}^3}|\psi(x,t)|^{\frac{8}{3}}\,dx$$

$$=C+\int_\xi^t\left(s\int_{\mathbb{R}^3}V(x,s)\,n(x,s)\,dx-\frac{3}{2}\,C_S s\int_{\mathbb{R}^3}|\psi(x,s)|^{\frac{8}{3}}\,dx\right)ds, \quad (30)$$

where

$$C=\|(x+i\xi\nabla)\,\psi(\cdot\,,\xi)\|^2_{L^2(\mathbb{R}^3)}+\xi^2\int_{\mathbb{R}^3}|\nabla V(x,\xi)|^2\,dx-\frac{3}{2}\,\xi^2 C_S\int_{\mathbb{R}^3}|\psi(x,\xi)|^{\frac{8}{3}}\,dx \quad (31)$$

and $\xi\geqslant 0$. Notice that this constant can be chosen positive if ξ is small enough because the right-hand side in (31) goes to $\|x\phi\|^2_{L^2(\mathbb{R}^3)}$ as $t\to 0$. Let $g(t)=t^2\int_{\mathbb{R}^3}Vn\,dx-\frac{3}{2}\,C_S t^2\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\,dx$. Then, from (30) we deduce

$$g(t)\leqslant C+\int_\xi^t\frac{g(s)}{s}\,ds.$$

Now Gronwall's lemma yields

$$g(t)=t^2\int_{\mathbb{R}^3}Vn\,dx-\frac{3}{2}\,C_S t^2\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\,dx\leqslant\frac{Ct}{\xi}\equiv C_\xi t,\qquad \forall t\geqslant\xi,$$

and we are done with the proof. ∎

Consider the function

$$f_\psi(t)=\|(x+it\nabla)\,\psi(\cdot\,,t)\|^2_{L^2(\mathbb{R}^3)}+t^2\int_{\mathbb{R}^3}|\nabla V(x,t)|^2\,dx-\frac{3}{2}\,C_S t^2\int_{\mathbb{R}^3}|\psi(x,t)|^{\frac{8}{3}}\,dx.$$

From (29) we get

$$f_\psi(t)\leqslant C+\int_\xi^t\frac{C_\xi s}{s}\,ds\leqslant C_\xi t.$$

The evolution of f_ψ (more precisely, the evolution of its sign) implies qualitative differences in the behaviour of the associated solution. The following result provides a decay estimate for the potential energy in the attractive case or a weak decay property for some $L^{p,q}$-norms of the wave functions.

Corollary 3.5. If there exists $t_0 \in \mathbb{R}^+$ such that $f_\psi(t_0) < 0$, then $f_\psi(t) < 0$ for all $t \geqslant t_0$. Furthermore,

$$2E_{\mathrm{POT}}(\psi) \leqslant \left(\frac{f_\psi(t_0)}{t_0}\right)\frac{1}{t} < 0, \qquad \forall t \geqslant t_0.$$

Otherwise we have

$$\int_\xi^\infty \|\psi(s)\|_{L^p(\mathbb{R}^3)}^{\frac{4p}{3(p-2)}}\, ds \leqslant C, \qquad \forall p \in (2, 6],$$

where C is a positive constant depending on p, $\|\phi\|_{L^2}$, $\|x\phi\|_{L^2}$, and ξ.

Proof. The first part of the corollary is deduced by using similar arguments to those of Proposition 3.4, when taking $\xi = t_0$.

Setting $\psi_g(x,t) := \exp(-\frac{ix^2}{2t})\,\psi(x,t)$ we have

$$it\nabla\psi_g(x,t) = \exp\left(-\frac{ix^2}{2t}\right)(x + it\nabla)\,\psi, \tag{32}$$

which implies

$$f_\psi(t) = t^2\,\|\nabla\psi_g\|_{\mathrm{L}^2(\mathbb{R}^3)}^2 + t^2\int_{\mathbb{R}^3} V(x,t)\,n(x,t)\,dx - \frac{3}{2}\,C_{\mathrm{S}}t^2\int_{\mathbb{R}^3}|\psi(x,t)|^{\frac{8}{3}}\,dx.$$

In the case $f_\psi > 0$ we have

$$\|\nabla\psi_g\|_{\mathrm{L}^2(\mathbb{R}^3)}^2 + \int_{\mathbb{R}^3} V(x,t)\,n(x,t)\,dx - \tfrac{3}{2}\,C_{\mathrm{S}}\int_{\mathbb{R}^3}|\psi(x,t)|^{\frac{8}{3}}\,dx > 0. \tag{33}$$

On the other hand, we can rewrite (23) in the following form

$$\frac{d}{dt}\left(t\,\|\nabla\psi_g(\cdot,t)\|_{\mathrm{L}^2(\mathbb{R}^3)}^2 + 2tE_{\mathrm{POT}}(\psi)(t)\right) = -\|\nabla\psi_g(\cdot,t)\|_{\mathrm{L}^2(\mathbb{R}^3)}^2.$$

Integrating between $\xi > 0$ and $t > \xi$ yields

$$t\,\|\nabla\psi_g(\cdot,t)\|_{\mathrm{L}^2(\mathbb{R}^3)}^2 + 2tE_{\mathrm{POT}}(\psi)(t) = \frac{f_\psi(\xi)}{\xi} - \int_\xi^t \|\nabla\psi_g(\cdot,t)\|_{\mathrm{L}^2(\mathbb{R}^3)}^2. \tag{34}$$

Now, the left-hand side of (34) can be estimated by using (33), which gives

$$\int_\xi^t \|\nabla\psi_g(\cdot,t)\|_{\mathrm{L}^2(\mathbb{R}^3)}^2 \leqslant \frac{f_\psi(\xi)}{\xi}.$$

The proof concludes by noting that the L^p norm of ψ and ψ_g coincide, then we can apply the Gagliardo–Nirenberg inequality to ψ_g. ∎

Let us now prove some decay properties of the solutions in the case of nonnegative potential energy.

Proposition 3.6. Let $\phi \in \Sigma$ the initial data of the SPS system and let ψ be the corresponding solution. If the potential energy associated with ψ is nonnegative along the time evolution, then there exist constants $C > 0$ which depend on $\|\phi\|_{L^2(\mathbb{R}^3)}$ and $\|x\phi\|_{L^2(\mathbb{R}^3)}$ such that

$$\text{(i)}\quad \forall |t| \geqslant 1, \quad \forall p \in [2, 6], \quad \|\psi(\cdot, t)\|_{L^p(\mathbb{R}^3)} \leqslant \frac{C}{|t|^{\frac{3}{2}(\frac{1}{2}-\frac{1}{p})}},$$

$$\text{(ii)}\quad \forall |t| \geqslant 1, \quad \forall p \in [1, 3], \quad \|n(\cdot, t)\|_{L^p(\mathbb{R}^3)} \leqslant \frac{C}{|t|^{\frac{3}{2}(1-\frac{1}{p})}},$$

$$\text{(iii)}\quad \forall |t| \geqslant 1, \quad \forall p \in]3, \infty[, \quad \|V(\cdot, t)\|_{L^p(\mathbb{R}^3)} \leqslant \frac{C}{t^{(\frac{1}{2}-\frac{3}{2p})}},$$

$$\text{(iv)}\quad \forall |t| \geqslant 1, \quad \forall p \in]\tfrac{3}{2}, \infty[, \quad \|\nabla V(\cdot, t)\|_{L^p(\mathbb{R}^3)} \leqslant \frac{C}{t^{(1-\frac{3}{2p})}}.$$

Proof. The proof follows the steps of Proposition 3.4 and the arguments given in refs. 6 and 12.

Using (32) the pseudo-conformal law can be written as

$$t^2 \|\nabla\psi_g(\cdot, t)\|^2_{L^2(\mathbb{R}^3)} = C + \int_\xi^t \left(s \int_{\mathbb{R}^3} |\nabla V(x, s)|^2 \, dx - \frac{3}{2} C_S s \int_{\mathbb{R}^3} |\psi(s)|^{\frac{8}{3}} \, dx \right) ds$$
$$- t^2 \int_{\mathbb{R}^3} |\nabla V(x, t)|^2 \, n(x, t) \, dx + \frac{3}{2} C_S t^2 \int_{\mathbb{R}^3} |\psi(x, t)|^{\frac{8}{3}} \, dx.$$

Then, applying (29) and taking into account the nonnegativity of the potential energy we find

$$\|\nabla\psi_g(\cdot, t)\|^2_{L^2(\mathbb{R}^3)} \leqslant \frac{C'}{t\xi},$$

for all $t \geqslant \xi$, where $C' = C'(C, \xi) > 0$. Now, the Gagliardo–Nirenberg inequality (applied to ψ_g) allows to get (i) for $p \in [2, 6]$ and $a = 3(\frac{1}{2} - \frac{1}{p})$:

$$\|\psi(\cdot,t)\|_{L^p(\mathbb{R}^3)} = \|\psi_g(\cdot,t)\|_{L^p(\mathbb{R}^3)} \leqslant \gamma(p)\, \|\nabla\psi_g(\cdot,t)\|^a_{L^2(\mathbb{R}^3)}\, \|\psi_g(\cdot,t)\|^{1-a}_{L^2(\mathbb{R}^3)}$$
$$\leqslant \gamma(p)\, \|\nabla\psi_g(\cdot,t)\|^a_{L^2(\mathbb{R}^3)}\, \|\phi\|^{1-a}_{L^2(\mathbb{R}^3)} \leqslant \frac{C'}{t^{\frac{3}{2}(\frac{1}{2}-\frac{1}{p})}}.$$

(ii) is a consequence of $\|n(\cdot,t)\|_{L^p(\mathbb{R}^3)} = \|\psi(\cdot,t)\|^2_{L^{2p}}$, while (iii) can be deduced from the Hardy–Littlewood–Sobolev inequality and (ii):

$$\|V(\cdot,t)\|_{L^p(\mathbb{R}^3)} \leqslant C' \left\| \frac{1}{r} * n(\cdot,t) \right\|_{L^p(\mathbb{R}^3)} \leqslant C'\, \|n(\cdot,t)\|_{L^q(\mathbb{R}^3)}$$
$$\leqslant C' \frac{1}{t^{\frac{3}{2}(1-\frac{1}{q})}} \leqslant C' \frac{1}{t^{(\frac{1}{2}-\frac{3}{2p})}},$$

where $\frac{1}{q} = \frac{1}{p} + \frac{2}{3}$ and $q \in\,]1,3[$. The proof of (iv) is analogous to that of (iii). ▮

4. MINIMIZATION OF THE ENERGY IN THE ATTRACTIVE CASE

The aim of this section is to give some results concerning the asymptotic behaviour in time of solutions to the SPS system under the assumption of attractive interactions. In this case the energy functional reads

$$E[\psi] = \int_{\mathbb{R}^3} \left\{ \frac{1}{2} |\nabla\psi(x,t)|^2 - \int_{\mathbb{R}^3} \frac{|\psi(x,t)|^2\, |\psi(x',t)|^2}{8\pi\, |x-x'|}\, dx' - \frac{3}{4}\, C_S\, |\psi(x,t)|^{\frac{8}{3}} \right\} dx. \tag{35}$$

Using the same arguments developed before to bound the energy in the repulsive case and the inequality (5), it can be shown that this functional has a lower bound over the set $\{\psi \in H^1(\mathbb{R}^3);\ \|\psi\|_{L^2(\mathbb{R}^3)} = M\}$. In ref. 3 it was proved the existence of a minimizer ψ_M of the energy functional (35) in $H^1(\mathbb{R}^3)$ under the constraint $\|\psi\|_{L^2(\mathbb{R}^3)} = M$, $M \in \mathbb{R}^+$. Furthermore, this minimum was found to be spherically symmetric. The proof given above can be also adapted to this case, therefore it might give an alternative way to obtain the existence of a minimum. In this case the restriction on the L^2-norm is not necessary because the potential energy is always negative.

Theorem 4.1. For all $M > 0$ there exists a minimizer $\psi_M \in C^\infty(\mathbb{R}^3)$ of the problem

$$\min\{E[\psi];\ \psi \in H^1(\mathbb{R}^3),\ \|\psi\|_{L^2(\mathbb{R}^3)} = M\},$$

where $E[\psi]$ denotes the energy functional (35). Also, ψ_M satisfies the Euler–Lagrange equation

$$-\frac{1}{2}\Delta\psi_M - \frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{|\psi_M(x',t)|^2}{|x-x'|}\,dx'\,\psi_M - C_S\,|\psi_M|^{\frac{2}{3}}\psi_M = \beta\psi_M$$

in a distributional sense, for some $\beta < 0$.

As an immediate consequence we get the existence of stationary waves of the form $\psi(x,t) = e^{-i\beta t}\psi_M(x)$ and we can construct solutions of the same type than in Proposition 2.10 satisfying (14). Also, from the minimization of the total energy operator we can deduce the same bound for the kinetic energy as in (20).

The dispersion properties (in the positive energy case) as well as the dispersion and pseudo-conformal laws are also valid in this case. However, since the potential energy is always negative in the attractive case, the decay properties of the solutions are no longer verified.

It is also possible to study the asymptotic behaviour of the solutions at $t = 0$. Actually, this analysis is a straightforward adaptation of the techniques developed in ref. 6 and shall be omitted here.

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