Journal of Statistical Physics, Vol. 103, Nos. 5/6, 2001

A Variational Approach to the Schrödinger–Poisson System: Asymptotic Behaviour, Breathers, and Stability

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Received July 14, 2000; final October 31, 2000

In this paper a variational formulation of the three-dimensional Schrödinger–Poisson system is proposed with the aim of solving the open problem of the asymptotic behaviour in time of the solutions in the case of attractive Coulomb forces. A dispersive equation relating density and linear moment dispersions is found. Optimal bounds for the kinetic energy are obtained which leads to study the asymptotic behaviour in time for the solutions in the attractive case with positive energy. The description of the asymptotic behaviour properties of the solutions such as a the existence of *breathing* mode solution, i.e. a changing size oscillatory wave function, in the case of attractive potential with negative kinetic energy are also given. A study of the stability of stationary solutions is proposed using a Liapunov functional and also starting from a perturbation of an associated time-independent solution of the Schrödinger–Poisson equation (linear stability).

KEY WORDS: Schrödinger–Poisson system; asymptotic behaviour; Coulomb forces.

1. INTRODUCTION

Recent advances in technology design, in particular the progressive tendency to fabricate semiconductor devices with extremely small sizes, have obliged to account for quantum-mechanical and numerical methods in order to describe quantum effects such as tunneling, size quantization or

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0022-4715/01/0600-1069$19.50/0

quantum interference. In this direction, Schrödinger–Poisson's system constitutes, since the early eighties, a quite extended mathematical framework to understand and analyze mathematical aspects which may prove relevant for the study of semiconductor heterostructures modeling. We refer to ref. 20 for a general setting of this and related models. The attractive case, which is our major concern in this paper, is also of interest in applications related to quantum gravity[6, 11, 26] in the limit of very heavy particles (known as the Schrödinger–Newton system in this context). In subsequent studies the stationary solutions of non-linear SP system have been stressed, either from a numerical,[28] analytical[22] or variational[12] viewpoint. For instance,[27] proves that a quantum heavy particle subjected to its own gravitational field becomes a black-hole as the particle mass approaches Planck's scale. Also, the attractive case is important in the quantum evolution of electrons in an ionic crystal (polaron) in the limit of high frequency optical phonons.[1]

The single particle Schrödinger–Poisson system governs the temporal evolution of the pure quantum-mechanical state wave function $\psi(x, t)$, which describes the state of a non- relativistic quantum particle in the coordinate space under the action of the self-consistent potential V originated by its own charge. In the attractive case, the Schrödinger–Poisson system describes the propagation in time of an electron in a polar crystal (a polaron), in the approximation for which the lattice vibrations or phonon cloud behave classically (strong coupling or mean field limit). The Schrödinger equation in $\mathbb{R}^3 \times (0, \infty)$ can be written as follows

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

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

when associated with a single particle system in vacuum, where $\hbar$ denotes Planck's constant and m the mass of the particle. To determine V we couple this system to the Poisson equation

$$\Delta_x V = -\gamma |\psi|^2, \qquad \lim_{|x| \to \infty} V = 0, \tag{3}$$

where $|\psi(x, t)|^2$ is the expected particle density for a pure quantum state in the position space $\mathbb{R}^3_x$ at time t and $\gamma = +1$ or $\gamma = -1$ depending on the repulsive or attractive character of the Coulomb force, respectively. The self-consistent potential V, solution of (3), can be explicitly written as

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

In this paper we are concerned with the study of the behaviour in time

of the wave function ψ, solution to the 3-D Schrödinger–Poisson system (SPS). Actually, we are interested in giving an insight on the quantum mechanical dynamics of a single particle in vacuum or a polar crystal (the polaron problem), and elucidating about its qualitative behaviour depending on the repulsive or attractive sign of the self-consistent Poisson potential, which to the best of our knowledge has been by no means completely well-understood through the literature and it constitutes an open problem in the attractive case until present. In this direction it is remarkable the contribution by Choquard to the quantum attractive modeling, discussed in ref. 16 by E. H. Lieb, where a description of an electron trapped in its own hole is given through an approximation to the Hartree–Fock theory for a one-component plasma: In particular, he proves existence and uniqueness of a minimizing solution to the energy functional associated with a Schrödinger–Poisson problem. This minimizing solution is proved to satisfy a stationary Schrödinger–Poisson equation. Related to the asymptotic behaviour in time of the solutions to the SPS under repulsive potential, let us mention the work of R. Illner, P. F. Zweifel and H. Lange[10] where it is proved that the wave function converges in the repulsive case to zero in L^p norm, $p > 2$, for large times when the initial data is in $H^2(\mathbb{R}^3)$. Also in the repulsive case, R. T. Glassey[7] showed that the particle density cannot be localized for large times inside a ball of any arbitrary radius, since it asymptotically vanishes provided that the solution has finite energy. The same result as in ref. 10 was extended by F. Castella to initial data in L^2 for the repulsive and attractive cases but under the hypothesis of infinite kinetic energy. These results show a "gap" in the theory of the asymptotic behaviour in time of solutions to the SPS in the attractive case with finite (positive or negative) energy.

From other point of view, in ref. 18 and 19, J. L. López and J. Soler analyzed the asymptotic behaviour for the 3-D SP system proving that the potential $tV(tx, t)$ tends to the Coulomb potential $V_\infty(x) = \frac{\gamma}{4\pi|x|}$ for large times. This type of behaviour is also found for finite time and $|x| \to \infty$. Motivated by this result and in order to gain some insight into the above open problems we try to characterize an approximate solution ψ^A by a localized shape, with finite L^2-norm and energy, and with spatial extension $R(t)^2$. Thus, we propose an easiest ansatz whose form is motivated by the Hydrogen-like asymptotic behaviour of the exact problem at large distances and take into account the invariants of the SPS (see Section 2). Due to the translational invariance of the Action functional associated to the SPS we can, without loss of generality, set the approximate solution localized at the origin of our coordinate axis, $\langle x \rangle(t) = 0$. Moreover, based on the Galilean invariance of $R(t)$ (Lemma 2.1), we can always choose our

reference frame as following the motion of the wave packet, i.e. that "at rest" where the mean momentum vanishes, $\langle p \rangle(t) = 0$. Since we have some freedom to fix the phase of the wave function, we will take the initial condition $\psi^A(x, 0)$ to be real. Then, the easiest ansatz suggested by the Hydrogen-like asymptotic behaviour we can think of is of the form $\psi^A(x, t) = A(t)\, e^{-\alpha(t) r} e^{i\beta(t) r}$, where $r = |x|$ and $A(t)$, $\alpha(t)$ and $\beta(t)$ are real functions. Imposing to this ansatz the conservation laws of the SP solutions, we find an ordinary differential equation for $R(t)$. The following curves (Fig. 1) represent the dependence of the energy $E(R)$ over the Lieb stationary energy E_L, $E(R)/E_L$, upon R/R_L in both repulsive and attractive cases, where R_L is the extension associated with the Lieb stationary solution. This figure shows that if the initial energy is positive $E(0) > 0$, the motion of the system is unbounded for both repulsive and attractive cases. The curves also give that the unbounded growth of the system is not possible when the initial energy is negative due to the energy preservation. If we plot the density as a function of time we see a localized solution whose width slightly oscillates in time. We may call this a *breathing* mode. Note that the results suggested by this ansatz agree with those of ref. 7 and 10 in the repulsive case and with those of ref. 4 for the repulsive and attractive cases with infinite positive energy. At large times, we have $R(t) \sim t^{2/3}$. Thus, for our approximate solution we obtain $\|\psi^A(\cdot, t)\|_{L^6(\mathbb{R}^3)} \sim t^{-2/3}$, bound which differs from that given by Castella in ref. 4 in $t^{-1/6}$ orders of magnitude.

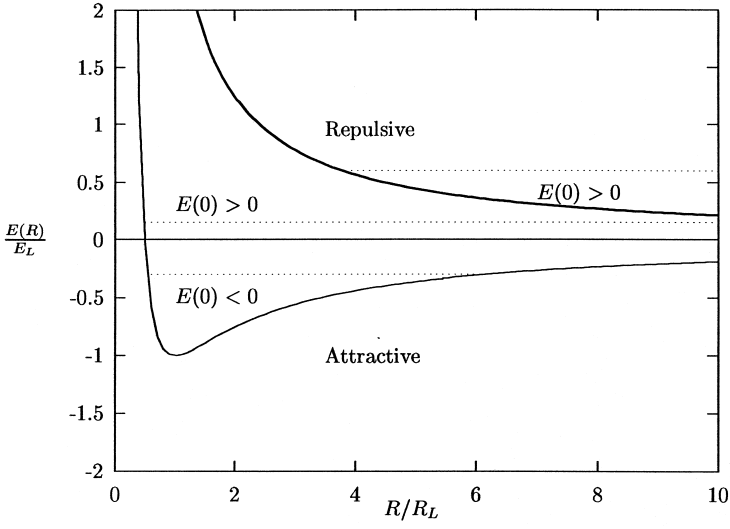

Fig. 1. Dependence of the energy $E(R)$ upon the extension R.

The aim of this paper is to try to corroborate the qualitative results suggested by the Fig. 1 with special attention on the attractive case with finite energy whose asymptotic analysis in time have not been discussed in the previous literature.

Let us summarize the techniques used through this paper as well as how it is organized. Our analysis relies first on a variational approach based on Noether's theorem, which formally describes the connection between invariance properties of the Action functional associated with the Schrödinger–Poisson operator and the corresponding physical quantities preserved through the temporal evolution, namely the motion invariants (see, for instance, ref. 8). In particular, the total mass, linear and angular momentum, total energy and boost operators contributing to the Schrödinger–Poisson system are deduced to be time-preserved in Section 2. The Poisson Bracket arguments allow to find that the invariants form a closed algebra, isomorphic to the Lie algebra of the generators of the Galilei group.

As a consequence of these preservation properties it is shown in Section 3 that the system remains unaccelerated during the evolution, i.e. the particle evolves with a constant velocity. This is in agreement with the particle interpretation of the solution since the system is moving in the absence of external forces. Also, a measure for the time variation of the wave packet size is proved in terms of the linear momentum variance via the derivation of a dispersive equation (see Eq. (27) below) in which the total energy operator is also involved. Some consequences are also extracted from this equation in the repulsive case.

In Section 4 we obtain optimal bounds on the kinetic energy in terms of the energy associated to the Lieb stationary solution which allows to deduce the asymptotic behaviour to the solutions of the SPS in the attractive case with positive energy. To do that the stationary Schrödinger–Poisson system is considered by analyzing the variational approach given by E. H. Lieb in ref. 16 and comparing the scaling properties of the solution and the energy with respect to the physical constants.

In Section 5, we study the analysis of stability of the Schrödinger–Poisson system for slightly perturbed oscillatory solutions around an equilibrium stationary solution. We introduce a Liapunov functional to study this problem and also the stability is discussed in terms of the sign of the relative frequencies of oscillations (linear stability).

Finally, Section 6 is devoted to the analysis of the attractive case with negative energy. We prove rigorously the existence of a bifurcating branch from the Lieb solution of breather mode solutions, i.e. changing size oscillatory density functions. The result agrees with the oscillatory character of solutions suggested in Fig. 1. The mathematical difficulty of the

problem is that in the attractive case the energy functional is not convex. The techniques are based on variational principles and in the use of the rearrangements of the wave functions which are related to the Lieb[16] techniques to deduce the minimal energy solution and on the works of Berger[2] about periodic solutions in dynamical systems.

Most of our presentation is done for the single state. It would be interesting to extend the present result to the mixed case, but this will require some additional effort which is beyond the purpose of the present work.

A variational formulation of the time-independent Schrödinger–Poisson problem was previously proposed by F. Nier in ref. 24 under quite different motivations. In particular, he proves existence and uniqueness of solutions to the Dirichlet problem in a bounded domain and also to the whole space problem when a periodic potential is considered, by transforming the Schrödinger–Poisson system into a minimization problem through a variational framework.

2. A VARIATIONAL FORMULATION. PROPERTIES

In this section we set the fundamentals of our variational approach and analyze the invariant action on the system of Galilei symmetry group, consisting of space and time translations, rotations and Galilei transformations or changes of inertial reference frames. As a consequence, the temporal invariance of the expected value of some related physical operators is obtained.

Assume that we are in the context of solutions $\psi(x, t) \in H^1(\mathbb{R}^3)$ for which the time integrals below make sense. Then, the Action functional associated with the Schrödinger–Poisson system can be written as follows

$$\begin{aligned}\mathscr{S}(\psi, \bar{\psi}) &= \int_0^\infty \int_{\mathbb{R}^3} \left\{ i\hbar\bar{\psi}\frac{\partial\psi}{\partial t} - \frac{\hbar^2}{2m}|\nabla_x\psi|^2 - V|\psi|^2 + \frac{1}{2\gamma}|\nabla_x V|^2 \right\} d(x, t) \\ &= \int_0^\infty \int_{\mathbb{R}^3} \left\{ i\hbar\bar{\psi}\frac{\partial\psi}{\partial t} - \frac{\hbar^2}{2m}|\nabla_x\psi|^2 - \frac{1}{2}V|\psi|^2 \right\} d(x, t). \end{aligned} \tag{5}$$

Then, taking into account the elliptic relation (4) connecting the potential and the wave function, the Action functional takes the form

$$\begin{aligned}\mathscr{S}(\psi, \bar{\psi}) = \int_0^\infty \int_{\mathbb{R}^3} \Bigg\{ & i\hbar\bar{\psi}(x, t)\frac{\partial\psi}{\partial t}(x, t) - \frac{\hbar^2}{2m}|\nabla_x\psi|^2(x, t) \\ & - \frac{\gamma}{8\pi}\int_{\mathbb{R}^3} \frac{|\psi(x, t)|^2\,|\psi(x', t)|^2}{|x - x'|}\,dx' \Bigg\} d(x, t). \end{aligned} \tag{6}$$

There exists a procedure for associating an energy equation with a variational principle. Noether's theorem (see e.g. refs. 8 and 9) shows that there is a conservation (volume integrated) equation corresponding to any continuous group of transformations for which the variational principle is invariant. Thus, the search of all conserved quantities is reduced to study the complete symmetry group of the Action functional. This is the real strength of Noether's theorem compared to the customary method consisting of deriving integral constants of motion by multiplying the equation by a suitable function and integrating. Although the application of Noether's theorem is well-known within Classical and Quantum Field Theory, we review here the main aspects which are relevant for the SPS. Due to the nonlinear character of the Schrödinger–Poisson operator, if we consider the group of invariant linear and unitary transformations for ψ in the Action associated with the SPS, this will be bounded by the maximal invariance group for the free Schrödinger equation, see U. Niederer.[23]

2.1. Invariances of the Action functional

Let us study invariances of the Action $\mathscr{S}$ under some groups of transformations and the corresponding preservation properties via Noether's theorem. The proof of the following results are derived from classical calculations.

Lemma 2.1. The following invariances and conservation laws are verified.

invariances	conservation laws
change of phase	total mass
$\psi(x, t) \to e^{i\alpha}\psi(x, t)$	$M = \int_{\mathbb{R}^3} \lvert\psi(x, t)\rvert^2 \, dx$
space translations	linear momentum
$\psi(x, t) \to \psi(x-a, t)$	$P(t) = \frac{\hbar}{i} \int_{\mathbb{R}^3} \bar{\psi}(x, t) \nabla_x \psi(x, t) \, dx$
rotations	angular momentum operator
$\psi(x, t) \to \psi(R^{-1}x, t)$	$J(t) = \frac{\hbar}{i} \int_{\mathbb{R}^3} \bar{\psi}(x, t)(x \wedge \nabla_x) \, \psi(x, t) \, dx$

time translations	total energy
$\psi(x, t) \to \psi(x, t-\tau)$	$E(t) = \int_{\mathbb{R}^3} \left\{ \frac{\hbar^2}{2m} \lvert \nabla_x \psi \rvert^2 (x, t) + \frac{\gamma}{8\pi} \int_{\mathbb{R}^3} \frac{\lvert \psi(x, t) \rvert^2 \lvert \psi(x', t) \rvert^2}{\lvert x - x' \rvert} dx' \right\} dx$
inertial frame change	boost operator (generator of the pure Galilei transformations)
$\psi(x, t) \to e^{i/\hbar(mv \cdot x - 1/2mv^2 t)} \psi(x - vt, t)$	$K(t) = t \frac{\hbar}{i} \int_{\mathbb{R}^3} \bar{\psi}(x, t) \nabla_x \psi(x, t) dx - m \int_{\mathbb{R}^3} \bar{\psi}(x, t) x \psi(x, t) dx$

All these symmetries are also symmetries for the free problem, i.e. the case with $V = 0$, and yield ten conserved quantities. However, there are two other invariances associated with the free problem which are not symmetries for the interacting case, namely conformal transformations and time-space dilatations[23] and which will be important in the rest of the paper.

Lemma 2.2. The Action functional $\mathscr{S}$ is not invariant under mass-preserving time-space dilatations, i.e. under transformations of type

$$\psi(x, t) \to \psi_\lambda(x, t) = \lambda^{3/2} \psi(\lambda x, \lambda t) \tag{7}$$

$$V(x, t) \to V_\lambda(x, t) = \lambda V(\lambda x, \lambda t), \tag{8}$$

for every $\lambda > 0$. In fact, we have that the Action $\mathscr{S}$ is mapped into $\mathscr{S}_\lambda$ under the transformation (7)–(8), where

$$\mathscr{S}_\lambda = \int_0^\infty \int_{\mathbb{R}^3} \left\{ i\hbar \bar{\psi}_\lambda(x, t) \frac{\partial \psi_\lambda}{\partial t} (x, t) - \lambda^{-1} \frac{\hbar^2}{2m} \lvert \nabla_x \psi_\lambda \rvert^2 (x, t) - \frac{\gamma}{8\pi} \int_{\mathbb{R}^3} \frac{\lvert \psi_\lambda(x, t) \rvert^2 \lvert \psi_\lambda(x', t) \rvert^2}{\lvert x - x' \rvert} dx' \right\} d(x, t). \tag{9}$$

Lemma 2.3. The Action functional $\mathscr{S}$ is not invariant under conformal transformations, i.e. under transformations of type

$$\psi(x, t) \to \psi_\xi(x, t) = (1 - \xi t)^{3/2} e^{-i(m \lvert x \rvert^2 \xi)/(2(1-\xi t))} \psi\left(\frac{x}{1 - \xi t}, \frac{t}{1 - \xi t} \right) \tag{10}$$

$$V(x, t) \to V_\xi(x, t) = (1 - \xi t)^5 V\left(\frac{x}{1 - \xi t}, \frac{t}{1 - \xi t} \right), \tag{11}$$

for every $\xi \in \mathbb{R}$. In fact, we have that the Action $\mathscr{S}$ is mapped into $\mathscr{S}_\xi$ under the conformal transformation (10)–(11), where

$$\begin{aligned}\mathscr{S}_\xi = \int_0^\infty \int_{\mathbb{R}^3} \Bigg\{ & \frac{1}{(1-\xi t)^5}\, i\hbar \bar{\psi}_\xi(x,t)\, \frac{\partial \psi_\xi}{\partial t}(x,t) \\ & - \frac{1}{(1-\xi t)^5} \frac{\hbar^2}{2m} |\nabla_x \psi_\xi|^2 (x,t) \\ & - \frac{1}{(1-\xi t)^{12}} \frac{\gamma}{8\pi} \int_{\mathbb{R}^3} \frac{|\psi_\xi(x,t)|^2\, |\psi_\xi(x',t)|^2}{|x-x'|}\, dx' \Bigg\} d(x,t) \\ & + \int_0^\infty \int_{\mathbb{R}^3} \frac{1}{(1-\xi t)^6} \Bigg\{ \Bigg(\frac{3}{2} i\hbar\xi + \frac{\hbar}{2} m\xi^2 x^2 \frac{1}{1-\xi t} \\ & - \frac{\hbar^2}{2} m\xi^2 x^2 \frac{1}{1-\xi t} \Bigg) |\psi_\xi|^2 (x,t) - i\hbar\xi \bar{\psi}_\xi(x,t)(x\cdot\nabla_x)\, \psi_\xi(x,t) \\ & + \mathrm{Re}\,(i\hbar^2 \xi \bar{\psi}_\xi(x,t)(x\cdot\nabla_x)\, \psi_\xi(x,t)) \Bigg\} d(x,t). \end{aligned} \tag{12}$$

The total energy preservation was formulated (in a weak sense) for mild H^2-solutions by R. Illner, P. F. Zweifel and H. Lange in ref. 10, Proposition 3.7. It is also remarkable that the pseudo-conformal conservation identity (see ref. 10)

$$\begin{aligned} & \|(x + it\nabla_x)\, \psi(\cdot, t)\|^2_{L^2(\mathbb{R}^3)} + t^2 \|\nabla_x V(\cdot, t)\|^2_{L^2(\mathbb{R}^3)} \\ & \qquad = \|x\varphi\|^2_{L^2(\mathbb{R}^3)} + \int_0^t s\, \|\nabla_x V(\cdot, s)\|^2_{L^2(\mathbb{R}^3)}\, ds. \end{aligned} \tag{13}$$

is still valid for weak L^2-solutions, as proved by F. Castella,[4] in spite of the kinetic energy of the particle $\|\nabla_x \psi(\cdot, t)\|^2_{L^2(\mathbb{R}^3)}$ is not bounded, in that case, for any time and the particle instantaneously goes to infinity.

In addition to the above mentioned continuous symmetries which yield the Noether invariants, there are other discrete symmetries[15] such as reflection symmetry, time reversal and charge conjugation (the latter includes changing the sign of the particle mass, m, also). It is also noteworthy that these invariance properties of the Action functional together with the uniqueness of the solution could have powerful consequences when regarding solutions corresponding to initial conditions which are invariant under some subgroup of the group of invariant transformations. We will illustrate this in the next section for the simple case of a real initial condition.

2.2. The Poisson Bracket Structure

It is interesting to realize that the SPS derived from the Action functional in (6) admits a Poisson bracket structure. Poisson structures are very well known in field theory, see ref. 25. The Poisson bracket of two functionals of ψ and $\bar{\psi}$, $\mathscr{A}$ and $\mathscr{B}$ is defined as

$$\{\mathscr{A}, \mathscr{B}\} = i \int_{\mathbb{R}^3} (\mathscr{A}_{\bar{\psi}(x,t)} \mathscr{B}_{\psi(x,t)} - \mathscr{B}_{\bar{\psi}(x,t)} \mathscr{A}_{\psi(x,t)})\, dx, \tag{14}$$

where $\mathscr{B}_{\psi(x,t)}$ indicates the (functional) Frechet derivative of the functional $\mathscr{B}$ with respect to $\psi(x, t)$ and where we take the rule $\psi(x, t)_{\psi(x',t)} = \delta(x - x')$ in a distributional sense. This definition is a simple generalization of the classical mechanics analog (see ref. 8), but taking into account that the field canonically conjugated to $\psi(x, t)$ (which plays the role of a coordinate) is $i\bar{\psi}(x, t)$. This Poisson bracket enjoys the properties of being i) bilinear in $\mathscr{A}$ and $\mathscr{B}$, ii) antisymmetric and iii) satisfying Jacobi's identity

$$\{\{\mathscr{A}, \mathscr{B}\}, \mathscr{C}\} + \{\{\mathscr{C}, \mathscr{A}\}, \mathscr{B}\} + \{\{\mathscr{B}, \mathscr{C}\}, \mathscr{A}\} = 0. \tag{15}$$

For an arbitrary functional one has the derivation rule

$$i\hbar \frac{d}{dt} \mathscr{A} = i\hbar \frac{\partial \mathscr{A}}{\partial t} + \{E, \mathscr{A}\}, \tag{16}$$

where E is the energy functional. For the particular case of bilinear functionals, which can be written as a scalar product $\mathscr{A} = \langle \psi |\, O_{\mathscr{A}} \,| \psi \rangle$ and $\mathscr{B} = \langle \psi |\, O_{\mathscr{B}} \,| \psi \rangle$ with $O_{\mathscr{A}}$ and $O_{\mathscr{B}}$ being self-adjoint operators we have $\{\mathscr{A}, \mathscr{B}\} = \langle \psi |\, [O_{\mathscr{A}}, O_{\mathscr{B}}] \,| \psi \rangle$, where $[O_{\mathscr{A}}, O_{\mathscr{B}}] = O_{\mathscr{A}} O_{\mathscr{B}} - O_{\mathscr{B}} O_{\mathscr{A}}$ is the quantum mechanical commutator and $\langle \beta_1 |\, O \,| \beta_2 \rangle$ means the matrix element $\langle \beta_1 |\, O \,| \beta_2 \rangle = \int_{\mathbb{R}^3} \bar{\beta}_1 (O\beta_2)\, dx$.

Then, the Poisson bracket structure of the Schrödinger–Poisson system takes the form

$$\mathscr{S}_{\bar{\psi}(x,t)} = i\hbar\, \partial_t \psi(x, t) - E_{\bar{\psi}(x,t)} = i\hbar\, \partial_t \psi(x, t) - \{E, \psi(x, t)\} = 0. \tag{17}$$

The complex conjugate equation is equivalent to this one since $E[\psi, \bar{\psi}] = E[\bar{\psi}, \psi]$.

A classical theorem of these Poisson structures is that if a functional $\mathscr{A}$ does not depend explicitly on time, then $\mathscr{A}$ is a constant of motion if and only if its Poisson bracket with the energy functional vanishes, i.e. $\{E, \mathscr{A}\} = 0$. Moreover, if two functionals $\mathscr{A}$ and $\mathscr{B}$ are constants of motion, then their Poisson bracket $\{\mathscr{A}, \mathscr{B}\}$ is also a constant of motion, see

ref. 13 and 25. As we have seen, there are eleven constants of motion M, E, $\vec{P}$, $\vec{J}$, $\vec{K}$. Notice that besides the energy functional E all others are bilinears in ψ and $\bar{\psi}$. The non-vanishing Poisson brackets of these conserved quantities are

$$\{K_i, J_j\} = i\hbar\varepsilon_{ijk}K_k, \qquad \{E, K_i\} = i\hbar P_i,$$
$$\{P_i, J_j\} = i\hbar\varepsilon_{ijk}P_k, \qquad \{P_i, K_j\} = i\hbar\,\delta_{ij}M,$$
$$\{J_i, J_j\} = i\hbar\varepsilon_{ijk}J_k,$$

where ε_{ijk} and δ_{ij} are the Levi–Civitta and the Kronecker coefficients, respectively. Therefore, no new conserved quantities originated by Poisson brackets exist. Then, we have shown the following result.

Proposition 2.1. The constants of motion M, E, $\vec{P}$, $\vec{J}$, $\vec{K}$ of the SPS form a closed algebra, isomorphic to the Lie algebra of the generators of the Galilei group, with the norm functional M playing the role of the inertial mass of the particle.

3. A DISPERSION EQUATION

In order to simplify the notation and from now on in the rest of the paper let us normalize the Planck constant to the unity.

Let us establish the following notation for the expectation value of f

$$\langle f\rangle(t) = \langle f(x, t), \psi(x, t)\rangle \overset{def}{=} \int_{\mathbb{R}^3} \bar{\psi}(x, t)\, f(x, t)\, \psi(x, t)\, dx, \tag{18}$$

where f could be an integrable function $f\colon \mathbb{R}^3 \times [0, \infty) \to \mathbb{R}^j$ or an operator acting on $\psi(x, t)$. Two special examples are the first order moment of the density (center of density), representing the expected value of the coordinate defined by

$$\langle x\rangle(t) = \int_{\mathbb{R}^3} \bar{\psi}(x, t)\, x\psi(x, t)\, dx \tag{19}$$

and the expected value of the linear momentum operator (quantity of mean modes)

$$P(t) = \langle p\rangle(t) \overset{def}{=} \left\langle \frac{1}{i}\nabla_x \right\rangle(t) = \frac{1}{i}\int_{\mathbb{R}^3} \bar{\psi}(x, t)\, \nabla_x\psi(x, t)\, dx. \tag{20}$$

In this section the calculations are done formally without taking care of regularity assumptions (the operators x and $p = i\nabla$ are unbounded).

However, it is not a problem at this point since the aim of the section is to show how estimates can be derived algebraically from the variational approach. The use of dilatation transformations is related to the Mourre theory based on the dilatations generator for the linear Schrödinger equation (see ref. 5).

It is a classical result in Quantum Mechanics (Ehrenfest's theorem), which can be deduced through a direct computation using the Schrödinger equation, the relationship

$$\frac{d}{dt}\langle x\rangle(t)=\frac{1}{m}\langle p\rangle(t). \tag{21}$$

Since the linear momentum is an invariant of motion (Noether's theorem, see Lemma 2.1) with respect to time, then the above equation (21) can be explicitly solved. We have proved the following result

Lemma 3.4. The center of density has the following linear growth in time

$$\langle x\rangle(t)=\frac{\langle p\rangle(0)}{m}\,t+\langle x\rangle(0). \tag{22}$$

This result states the simple fact that the extended solution $\psi(x, t)$ represents a particle with internal structure which moves in the absence of external forces. This equation is a simple consequence of the Galilean invariance of the system stated in Lemma 2.1.

For the sake of simplicity in future calculations and as a direct way to prove (21), we will use the classical bracket notation. Given two non-commutative operators associated with some physical quantities, let us denote by $[\,\cdot\,,\,\cdot\,]$ the usual quantum Poisson's bracket formalism defined by $[A, B]=i(AB-BA)$. Using the Hamiltonian operator associated with the Schrödinger equation $H=-\frac{1}{2m}\nabla_x^2+V=\frac{1}{2m}p^2+V$, we can easily deduce

$$\frac{d}{dt}\langle f\rangle(t)=\langle[H, f]\rangle(t)+\left\langle\frac{\partial}{\partial t}f\right\rangle(t). \tag{23}$$

Then, taking into account the equalities

$$[p, x]=I_3 \qquad \text{and} \qquad [H, x]=\frac{p}{m}, \tag{24}$$

it is straightforward to deduce (21), where I_3 is the identity matrix in $\mathbb{R}^{3\times 3}$ and where the following property of Poisson's brackets

$$[AB, C] = A[B, C] + [A, C]\, B \tag{25}$$

is used to deduce the second relation in (24).

In the following result we shall derive an equation relating the position and moment dispersions. A remarkable fact is that this equation is a distinctive feature of the Coulomb interaction, regardless of the quantum-mechanical underlying dynamics. It can be checked that this equation is also fulfilled for a system of classical charged particles or for its statistical limit, like occurs in the context of Vlasov–Poisson system. A predecessor of this equation was given by P. L. Lions and T. Paul in ref. 17 by means of the Wigner formulation. In fact, this dispersive equation can be considered as a direct derivation from the pseudoconformal law (13) studied in (10) and (4) and obtained here in a different and simpler form and go further by exploiting its consequences.

Let us denote by

$$R(t)^2 = (\Delta x)^2(t) \overset{def}{=} \langle x^2\rangle(t) - \langle x\rangle^2(t) \quad \text{and} \quad (\Delta p)^2(t) \overset{def}{=} \langle p^2\rangle(t) - \langle p\rangle^2(t). \tag{26}$$

Lemma 3.5. The following equation connecting the position and moment dispersions

$$\frac{d^2}{dt^2}(\Delta x)^2(t) = \frac{2}{m}\left(E(t) - \frac{1}{2m}\langle p\rangle^2(t)\right) + \frac{1}{m^2}(\Delta p)^2(t) \tag{27}$$

holds, $E(t)$ being the energy operator defined in, Lemma 2.1.

Proof. We first find the equation for the time derivatives of the second order moment of the density. Applying (23) with $f = x^2$, we have

$$\frac{d}{dt}\langle x^2\rangle(t) = \int_{\mathbb{R}^3} \bar{\psi}(x, t)[H, x^2]\, \psi(x, t)\, dx.$$

Using (25) and the homologous relation

$$[A, BC] = B[A, C] + [A, B]\, C, \tag{28}$$

we deduce

$$[p^2, x^2] = \sum_{j=1}^{3} \{p_j [p_j, x^2] + [p_j, x^2]\, p_j\} = 2(xp + px)$$

which implies, by using $[H, x^2] = \frac{1}{2m}[p^2, x^2]$,

$$\frac{d}{dt}\langle x^2 \rangle(t) = \frac{1}{m}\langle xp + px \rangle(t). \tag{29}$$

Taking into account (23) and (29), we have for the second derivative

$$\frac{d^2}{dt^2}\langle x^2 \rangle(t) = \frac{1}{m}\langle [H, xp + px] \rangle(t).$$

From (24) and (28) we get $[H, xp] = [H, px] = (\frac{1}{m} p^2 - x \cdot \nabla_x V)(t)$. Therefore,

$$\frac{d^2}{dt^2}\langle x^2 \rangle(t) = \frac{2}{m}\left\langle \frac{1}{m} p^2 - x \cdot \nabla_x V \right\rangle(t). \tag{30}$$

In order to give a closed expression for (30) in terms of the first and second order moments of momentum and density we evaluate $\langle x \cdot \nabla_x V \rangle$ with the help of (4) as follows

$$\begin{aligned}
\langle x \cdot \nabla_x V \rangle(t) &= \int_{\mathbb{R}^3} \bar{\psi}(x, t)\, x \cdot \nabla_x V(x, t)\, \psi(x, t)\, dx \\
&= \int_{\mathbb{R}^3} |\psi(x, t)|^2\, x \cdot \nabla_x \left(\frac{\gamma}{4\pi} \int_{\mathbb{R}^3} \frac{|\psi(x', t)|^2}{|x - x'|}\, dx' \right) dx \\
&= -\int_{\mathbb{R}^3} |\psi(x, t)|^2\, x \left(\frac{\gamma}{4\pi} \int_{\mathbb{R}^3} \frac{x - x'}{|x - x'|} |\psi(x', t)|^2\, dx' \right) dx,
\end{aligned}$$

that, due to the antisymmetry property of the kernel $x \frac{x - x'}{|x - x'|^3}$, gives

$$= -\frac{\gamma}{8\pi} \int_{\mathbb{R}^6} \frac{|\psi(x, t)|^2\, |\psi(x', t)|^2}{|x - x'|}\, dx'\, dx.$$

Now, the definition of the total energy (Lemma 2.1) allows to write

$$\langle x \cdot \nabla_x V \rangle = \frac{1}{2m} \int_{\mathbb{R}^3} \nabla_x \bar{\psi}(x, t)\, \nabla_x \psi(x, t)\, dx - E(t) = \frac{1}{2m}\langle p^2 \rangle(t) - E(t). \tag{31}$$

Hence, combining (30) and (31) we finally obtain

$$\frac{d^2}{dt^2}\langle x^2\rangle(t)=\frac{2}{m}\left\{\frac{1}{2m}\langle p^2\rangle(t)+E(t)\right\}. \tag{32}$$

Then, the announced result follows from (21) and (32). ▮

By easy calculations, the dispersion equation (27) gives

$$\frac{m}{2}\frac{d^2}{dt^2}\langle x^2\rangle=E_{KIN}+E(t), \tag{33}$$

which will be useful later in Section 6.

Let us now prove that equation (27) is an invariant for the Schrödinger–Poisson system. Define a Galilei transformation as in ref. 15

$$\psi(x, t)\to e^{-i(-mv\cdot x+1/2\,mv^2t)}\psi(x-vt, t), \qquad v\in\mathbb{R}^3.$$

Lemma 3.6. (i) The position dispersion $(\Delta x)^2(t)$ is a Galilei invariant.
(ii) The momentum dispersion $(\Delta p)^2(t)$ is also a Galilei invariant.

Proof. The first order moment of the density becomes

$$\begin{aligned}\langle x, \psi(x-vt, t)\rangle&=\int_{\mathbb{R}^3}\bar{\psi}(x-vt, t)\, x\psi(x-vt, t)\, dx\\ &=\int_{\mathbb{R}^3}|\psi(x, t)|^2\,(x+vt)\, dx=\langle x\rangle(t)+vt\end{aligned} \tag{34}$$

under Galilei transformations. In the same way, for the second order moment of the density we have

$$\langle x^2, \psi(x-vt, t)\rangle=\langle (x+vt)^2\rangle(t)=\langle x^2\rangle(t)+v^2t^2+2vt\langle x\rangle(t). \tag{35}$$

Then, as a consequence of (34) and (35), the mean square deviation for the coordinate $(\Delta x)^2(t)$ verifies

$$(\Delta x, \psi(x-vt, t))^2\overset{def}{=}\langle x^2, \psi(x-vt, t)\rangle-\langle x, \psi(x-vt, t)\rangle^2=(\Delta x)^2\,(t),$$

which gives its invariance under Galilei transformations.

Analogously, concerning with the mean square deviation for the linear momentum we can write

$$\langle p, \psi(x-vt, t)\rangle = \frac{1}{i}\int_{\mathbb{R}^3} \overline{(e^{-i(-mv\cdot x+1/2\, mv^2 t)}\psi(x-vt, t))} \times \nabla_x (e^{-i(-mv\cdot x+1/2\, mv^2 t)}\psi(x-vt, t))\, dx,$$

where we have applied the fact that if $(\psi(x, t), V(x, t))$ is a solution to the SPS, then the pair $(\exp\{i\phi(x, t)\}\psi(x, t), V(x, t))$ is also a solution for any real function Φ. Then, the mass preservation property (Lemma 2.1) gives

$$\langle p, \psi(x-vt, t)\rangle = \langle p\rangle(t) + mv. \tag{36}$$

A similar argument leads to

$$\langle p^2, \psi(x-vt, t)\rangle = \langle p^2\rangle(t) + (mv)^2 + 2mv\langle p\rangle(t). \tag{37}$$

Hence, combining both equations (36) and (37) we deduce that the momentum dispersion $(\Delta p)^2(t)$ also verifies

$$(\Delta p, \psi(x-vt))^2 \stackrel{def}{=} \langle p^2, \psi(x-vt, t)\rangle - \langle p, \psi(x-vt, t)\rangle^2 = (\Delta p)^2(t)$$

thus is a Galilei invariant. ▮

The above result can be generalized. In fact, all centered moments of the form $\langle (x-\langle x\rangle)^n\rangle$ and $\langle (p-\langle p\rangle)^n\rangle$ are Galilei invariant.

Let us remark that the dispersion equation (27) can be also deduced as a consequence of the stationary character of the Action functional under some transformations. In particular, we have the following result.

Lemma 3.7. The variation of the Action functional $\mathscr{S}$

(i) under dilatation transformations:

$$\psi(x, t) \to \psi_{\lambda(t)}(x, t) = \lambda^{3/2}(t)\, \psi(\lambda(t)\, x, t)$$
$$V(x, t) \to V_{\lambda(t)}(x, t) = \lambda(t)\, V(\lambda(t)\, x, t),$$

(ii) under conformal transformations:

$$\psi(x, t) \to \psi_\xi(x, t) = (1-\xi t)^{3/2}\, e^{-i\frac{m|x|^2\xi}{2(1-\xi t)}} \psi\left(\frac{x}{1-\xi t}, \frac{t}{1-\xi t}\right)$$

$$V(x, t) \to V_\xi(x, t) = (1-\xi t)^5\, V\left(\frac{x}{1-\xi t}, \frac{t}{1-\xi t}\right),$$

implies the dispersion equation (27).

Proof. The dilatation $\psi(x, t) \to \psi_{\lambda(t)}(x, t) = \lambda^{3/2}(t)\, \psi(\lambda(t)\, x, t)$ provides

$$\mathscr{S}(\psi_{\lambda(t)}, \bar{\psi}_{\lambda(t)}) = \int_0^\infty \left\{\frac{3}{2} i\lambda'(t)\left(\frac{1}{\lambda(t)} - 1\right) + i\langle \partial_t \rangle(t) \right.$$

$$\left. -\lambda'(t)\frac{m}{2}\frac{d}{dt}\langle x^2\rangle(t) - \frac{1}{2m}\lambda^2(t)\langle p^2\rangle(t) - \frac{1}{2}\lambda(t)\langle V\rangle(t)\right\} dt,$$

where we have used $\langle xp\rangle(t) = \frac{m}{2}\frac{d}{dt}\langle x^2\rangle(t) + \frac{3}{2} i$ as an easy consequence of (29).

Then, minimizing this variation with respect to $\lambda(t)$ around $\lambda(t) = 1$ we find

$$\frac{m}{2}\frac{d^2}{dt^2}\langle x^2\rangle(t) = \frac{1}{m}\langle p^2\rangle(t) + \frac{1}{2}\langle V\rangle(t) = \frac{1}{2m}\langle p^2\rangle(t) + E(t).$$

Subtracting from this formula the identity $\frac{m}{2}\frac{d^2}{dt^2}\langle x\rangle^2(t) = \frac{1}{m}\langle p\rangle^2(t)$, which is a direct consequence of (21) and the preservation of the linear momentum, we deduce the dispersion equation (27).

In a similar way, we can obtain (27) by using (10)– (11). ∎

A first consequence we can deduce from equation (27) is that for each real initial condition associated with the Schrödinger–Poisson system there corresponds linear momentum zero and an initial stationary dispersion. In fact, if φ is a real function we can write

$$\frac{d}{dt}\langle x^2\rangle(t)\Big|_{t=0} = \frac{1}{m}\frac{1}{i}\int_{\mathbb{R}^3} \{\varphi(x\cdot\nabla_x)\,\varphi + \varphi(\nabla_x\cdot x)\,\varphi\}\, dx.$$

Taking the conjugate complex we find

$$\overline{\frac{d}{dt}\langle x^2\rangle(t)\Big|_{t=0}} = -\frac{d}{dt}\langle x^2\rangle(t)\Big|_{t=0} \Rightarrow \frac{d}{dt}\langle x^2\rangle(t)\Big|_{t=0} = 0.$$

But, in this case, the moment is also zero because of

$$\langle p\rangle(0)=\langle p\rangle(t)=\frac{1}{i}\int_{\mathbb{R}^3}\varphi\,\nabla_x\varphi\,dx=\frac{1}{i}\frac{1}{2}\int_{\mathbb{R}^3}\nabla_x(\varphi^2)\,dx=0,$$

which implies from (22) $\langle x\rangle(t)=\langle x\rangle(0)$. In a similar way and using (27) we can also prove that, for a real initial condition,

$$\frac{d}{dt}\langle p^2\rangle(t)\Big|_{t=0}=0,\qquad \frac{d^3}{dt^3}\langle x^2\rangle(t)\Big|_{t=0}=0.$$

In fact, these properties regarding vanishing values of integral quantities at $t=0$ are a simple consequence of time reversal invariance, namely the invariance of the Schrödinger–Poisson system under the transformation $\psi(x,t)\to\bar{\psi}(x,-t)$, which means that if $\psi(x,t)$ is a solution corresponding to the initial condition $\varphi(x)$, then $\bar{\psi}(x,-t)$ is also a solution corresponding to the complex conjugated initial condition $\bar{\varphi}(x)$. If the initial condition is real, then by uniqueness of the solution we must have $\psi(x,t)=\bar{\psi}(x,-t)$. Thus, in particular $|\psi(x,t)|^2=|\psi(x,-t)|^2$ and, more generally, all bilinear integral and real quantities such as $\langle x^n\rangle(t)$ for all n, and $\langle p^n\rangle(t)$ for even n are even at time t, hence their derivatives of odd order identically vanish at $t=0$. Likewise, $\langle p^n\rangle(t)$ for odd n are odd in t and their even order derivatives vanish.

For the repulsive case it is then a simple matter to recover (see ref. 7 and 10) from (27) or (33) by using that the total energy is always positive the following result.

Proposition 3.2. In the repulsive case the dispersion is always a convex function of time. From here it follows an increasing dispersion in time, so that $\psi(x,t)$ spreads out as time grows.

No concluding results can be obtained from (33) in the attractive case. However under some hypothesis the same type of behaviour applies for the attractive case with positive initial energy. This can be achieved by letting $\langle x^2\rangle$ to become sufficiently small, since by the uncertainty relation $(\Delta x)^2(t)(\Delta p)^2(t)\geqslant\frac{9}{4}$ the kinetic energy $\langle p^2/2m\rangle$ becomes sufficiently large so as to dominate over the potential energy $-\langle V\rangle/2$. For negative initial energy, however, we can only deduce that $\frac{m}{2}\frac{d^2}{2}\langle x^2\rangle(t) > \inf E+\frac{1}{\langle x^2\rangle(t)}\frac{9}{8m}$ after an appropriate normalization.

Note that, since the energy functional takes its minimum at a negative value in this case, nothing prevents in principle from a change of convexity of the dispersion. Therefore, we can only obtain concluding results in the repulsive case while in the attractive case the results are only partially

satisfactory. However, Fig. 1 motivated us to improve the bounds for the kinetic energy to try to corroborate its suggested behaviour for the solutions.

4. BEHAVIOUR OF SOLUTIONS IN THE ATTRACTIVE CASE WITH POSITIVE ENERGY

The aim of this Section is to prove that if the initial energy is positive the system expands unboundedly. Let us first review some aspects concerning with the stationary case. If we start from a time independent density, we expect from the dispersion equation that at any time $E+\frac{1}{2m}\langle p^2\rangle=0$, thus the kinetic energy should become a constant of motion. A particular kind of solution corresponding to constant density in time is of the form $\psi(x, t)=e^{-iet}\psi(x)$, so that the Schrödinger–Poisson system reduces to the time-independent Schrödinger equation

$$\varepsilon\psi=-\frac{1}{2m}\Delta_x\psi+V\psi, \qquad \lim_{|x|\to\infty}\psi=0 \tag{38}$$

coupled to Poisson's equation (3). Clearly, if we take as initial condition a function $\psi(x)$ satisfying the previous set of equations, then the solution as a function of time is represented by the function $\psi(x, t)$. It is well-known that this problem can be formulated in a variational context, namely the solution is an extremal of the energy functional. Indeed, E. Lieb[16] proved that in the attractive case there is a unique L^2 solution minimizing the energy functional (referred to as Choquard's energy functional), the "eigenvalue" ε_L, associated to the Lieb solution, being the corresponding Lagrange multiplier. Furthermore, this solution was found to be spherically symmetric. Numerical investigation was also done to compute the numerical value to some desired accuracy. Notice that the above problem (38) enjoys some symmetries, namely invariance under phase transformations, space translations, rotations and boosts.

Some integral relations, usually called virial theorems, can be obtained from the stationarity of the energy with respect to particular variations upon $\psi(x)$ and $V(x)$. Multiplying the Schrödinger equation (38) by the wave function associated to the minimal Lieb solution $(\psi_L(x), V_L)$ and integrating we get, for normalized states, $\varepsilon_L=\frac{1}{2m}\langle p^2\rangle_L+\langle V_L\rangle_L$. The subscript L stands for the corresponding average with respect to the wave function $\psi_L(x)$. This yields

$$E_L=\frac{1}{2m}\langle p^2\rangle_L=\frac{1}{3}\varepsilon_L$$

as long as the stationary potential and kinetic energy verify

$$E^L_{KIN} = -\varepsilon_L/3 \qquad \text{and} \qquad E^L_{POT} = 2\varepsilon_L/3. \tag{39}$$

These relations are in fact necessary conditions for a solution to be a stationary one. Lieb's minimal energy can be conveniently written in terms of a positive dimensionless constant c, which can be evaluated numerically, as

$$E_L = -cm\left(\frac{5\gamma}{64\pi}\right)^2. \tag{40}$$

Another interesting aspect is to compare two problems with different values of the parameters, namely (m, γ) and (m_0, γ_0). This yields certain scaling relations which allow to compute all possible values (m, γ) in terms of some reference values (m_0, γ_0). The best way to derive them is to consider the energy functional $E(m_0, \gamma_0)[\varphi]$ with minimum $\psi_0(x)$ and the energy functional $E(m, \gamma)[\varphi]$ with minimum $\psi(x)$. We propose for the second problem $\varphi(x) = \lambda^{3/2}\psi_0(\lambda x)$. Now, minimizing with respect to λ we get

$$\psi(x) = \left(\frac{\gamma m}{\gamma_0 m_0}\right)^{3/2} \psi_0\left(\frac{\gamma m}{\gamma_0 m_0}\right).$$

Hence,

$$E(\gamma, m) = \left(\frac{m\gamma^2}{m_0\gamma_0^2}\right) E(\gamma_0, m_0) \tag{41}$$

and a similar relation for the eigenvalue $\varepsilon(\gamma, m)$, while for a time dependent solution becomes

$$\psi(x, t) = \left(\frac{\gamma m}{\gamma_0 m_0}\right)^{3/2} \psi_0\left(\frac{\gamma m}{\gamma_0 m_0} x, \frac{\gamma^2 m}{\gamma_0^2 m_0}\right).$$

The equations (39) and (41) also hold for any stationary solution. This relation will be applied later for $\psi_0 = \psi_L$.

Then, let us first deduce some optimal bounds for the energies.

Proposition 4.3. The kinetic energy associated to the solutions of the Schrödinger–Poisson system are bounded between the extremal optimal values $E^{\pm}_{KIN}$ given by

$$E^{pm}_{KIN} = -2E_L\left(1 - \frac{E_0}{2E_L} \pm \sqrt{1 - \frac{E_0}{E_L}}\right), \tag{42}$$

where E_0 is the initial energy and E_L is the energy of the Lieb solution.

Proof. Since the following estimates are valid for any time we drop the explicit time-dependence of the wave function. It is known that the interaction energy associated with mild solutions of the SPS can be bounded in terms of the kinetic energy in the form

$$\int_{\mathbb{R}^6} \frac{|\psi(x)|^2\,|\psi(x')|^2}{|x-x'|}\,dx'\,dx \leqslant C\left(\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx\right)^{1/2},$$

where C is a positive constant (see ref. 10). We optimize this bound by minimizing the functional

$$\mathscr{F}[\psi] = \frac{\displaystyle\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx}{\left(\displaystyle\int_{\mathbb{R}^6} \frac{|\psi(x)|^2\,|\psi(x')|^2}{|x-x'|}\,dx'\,dx\right)^2} > 0$$

on $L^2(\mathbb{R}^3)$ under the restriction $||\psi||_{L^2(\mathbb{R}^3)} = 1$. Then, the Euler–Lagrange equation associated with this functional reads

$$\frac{-\Delta\psi(x)}{\left(\displaystyle\int_{\mathbb{R}^6} \frac{|\psi(x)|^2\,|\psi(x')|^2}{|x-x'|}\,dx'\,dx\right)^2} - \frac{4\displaystyle\int_{\mathbb{R}^3} \frac{\psi(x)\,|\psi(x')|^2}{|x-x'|}\,dx'}{\left(\displaystyle\int_{\mathbb{R}^6} \frac{|\psi(x)|^2\,|\psi(x')|^2}{|x-x'|}\,dx'\,dx\right)^3} \int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx - \lambda\psi(x) = 0.$$

This problem can be rewritten as

$$-\frac{1}{2m_0}\Delta\psi_0(x) + \frac{\gamma_0}{4\pi}\left(\int_{\mathbb{R}^3} \frac{|\psi_0(x')|^2}{|x-x'|}\,dx'\right)\psi_0(x) = \varepsilon_0\psi_0(x), \tag{43}$$

which is similar to the stationary SPS (38). Identifying the parameters we have

$$\int_{\mathbb{R}^6} \frac{|\psi_0(x)|^2\,|\psi_0(x')|^2}{|x-x'|}\,dx'\,dx = 2m_0, \tag{44}$$

$$-4\,\frac{\displaystyle\int_{\mathbb{R}^3} |\nabla\psi_0(x)|^2\,dx}{\left(\displaystyle\int_{\mathbb{R}^6} \frac{|\psi_0(x)|^2\,|\psi_0(x')|^2}{|x-x'|}\,dx'\,dx\right)^2} = \frac{\gamma_0}{4\pi} \tag{45}$$

and

$$\lambda \int_{\mathbb{R}^6} \frac{|\psi_0(x)|^2 \, |\psi_0(x')|^2}{|x-x'|} \, dx' \, dx = \varepsilon_0 \equiv \varepsilon(\gamma_0, m_0).$$

Multiplying (43) by $\bar{\psi}_0$ and integrating over $\mathbb{R}^3$, we obtain

$$-3 \min \mathscr{F}[\psi] = -3\mathscr{F}[\psi_0] = \lambda. \tag{46}$$

Then, to determine λ we can evaluate the potential and kinetic energy as follows:

$$E_{POT}(\gamma_0, m_0) = \frac{\gamma_0}{8\pi} \int_{\mathbb{R}^6} \frac{|\psi_0(x)|^2 \, |\psi_0(x')|^2}{|x-x'|} \, dx' \, dx = \frac{\gamma_0 m_0}{4\pi} < 0$$

$$E_{KIN}(\gamma_0, m_0) = \int_{\mathbb{R}^3} \frac{|\nabla \psi_0(x)|^2}{2m_0} \, dx = \frac{-2\pi}{m_0 \gamma_0} E_{POT}^2(\gamma_0, m_0) = -\frac{\gamma_0}{8\pi} m_0 > 0,$$

where we have used (45). On the other hand, by using the stationary relations given in (39) we find $\varepsilon_0 = 3\gamma_0 m_0 / 8\pi$ and

$$\lambda = \frac{\varepsilon_0}{2m_0} = \frac{3\gamma_0}{16\pi} < 0. \tag{47}$$

There only remains to calculate γ_0 from the scale parameters. For that, using the scale relations (41) we have

$$\varepsilon_0 = \frac{3\gamma_0 m_0}{8\pi} = \frac{m_0 \gamma_0^2}{m\gamma^2} \varepsilon_L = -3c \left(\frac{5\gamma_0}{64\pi} \right)^2 m_0,$$

where c is the smallest eigenvalue. This implies

$$\gamma_0 = -\frac{1}{8\pi} \left(\frac{64\pi}{5} \right)^2 \frac{1}{c}. \tag{48}$$

Combining (46), (47) and (48) we obtain $2mc(\frac{5\gamma}{64\pi})^2 \, 2E_{KIN} \geqslant E_{POT}^2$, from which, using (40), we deduce the bound

$$E_{POT} \geqslant -\sqrt{-2E_L} \sqrt{2E_{KIN}}. \tag{49}$$

Since our minimum represents a stationary state, the total energy verifies

$$E_0 \overset{def}{=} E_{KIN} + E_{POT} \geqslant -cm \left(\frac{5\gamma}{64\pi} \right)^2 \equiv \inf E = E_L,$$

which is precisely the estimate for Lieb's solution (40). Now, using the energy conservation property together with (49), we find the inequality

$$E_{KIN} - \sqrt{-2E_L}\,\sqrt{2E_{KIN}} \leqslant E_{KIN} + E_{POT} = E_0$$

which yields

$$E_{KIN}^2 - 2E_0 E_{KIN} + E_0^2 \leqslant -4E_L E_{KIN}.$$

From this equation it is a simple matter to obtain (42) given in the Proposition statement. The bound $E \geqslant E_{KIN} - 2\sqrt{-E_L}\,E_{KIN}^{1/2}$ is sharp since minimizing the left hand side of the above inequality with respect to E_{KIN} we obtain $E_{KIN} = -E_L$ (virial theorem) and, hence, $E = E_L$. ∎

Now, combining the estimate for the kinetic energy given in the above Proposition together with the dispersive equation we find the announced main result:

Theorem 4.1. Let $\varphi \in H^1(\mathbb{R}^3)$ be the initial real condition of the SPS with a positive initial finite energy $0 < E_0 < \infty$ and finite initial dispersion $\langle x^2 \rangle(0) < \infty$. Then, the system expands unboundedly for large times and the dispersion $\langle x^2 \rangle(t)$ behaves like $O(t^2)$.

Proof. To deduce our result, let us write the dispersive equation in the form

$$\frac{m}{2}\frac{d^2}{dt^2}\langle x^2 \rangle = E_{KIN} + E_0$$

which implies by using (42) the following bounds

$$E_{KIN}^- + E_0 \leqslant \frac{m}{2}\frac{d^2}{dt^2}\langle x^2 \rangle \leqslant E_{KIN}^+ + E_0.$$

Hence, if $E_0 > 0$, both bounds are also positive which allows to find the result by integrating twice in time the equation; the system expands as $\langle x^2 \rangle \sim t^2$. ∎

The above estimate is sharp also from the following point of view: since the initial energy coincides with the Lieb infimum, $E_0 = E_L$, then both parts of the inequality vanish and $\langle x^2 \rangle$ remains constant. The former nested inequality is not very useful in the limit of large times in the attractive case, since the left hand side becomes negative, meaning that the system cannot contract too quickly, but for some finite time, this bound

becomes worse than Heisenberg's uncertainty principle, $\langle x^2\rangle\langle p^2\rangle \geqslant 9/4$, in the center of mass system. In this case, the right hand side only says that the system cannot expand faster than as predicted in the repulsive case.

Numerically we can obtain an approximation to the optimal constant that minimize the estimation of the potential energy in terms of the kinetic one, $\min \mathscr{F} = 5\sqrt{2c}/8 = 0.6588$, thus

$$\int_{\mathbb{R}^6} \frac{|\psi(x)|^2\,|\psi(x')|^2}{|x-x'|}\,dx'\,dx \leqslant 0.6588\left(\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,dx\right)^{1/2}$$

and the equality holds true for the Lieb solution.

5. STABILITY NEAR THE MINIMAL SOLUTION

The results in Fig. 1 suggest that under certain initial conditions of negative energy in the attractive case the behaviour of the solution might be oscillatory. In order to corroborate this property we will first try to describe the stability of the solutions which are close to the minimal Lieb stationary solution.

Let us first note that the energy acts like a Liapunov functional. In fact, the energy $E(t)$ plus the minimum of the energy $|\varepsilon_L|$ at the Lieb stationary solution is a nonnegative definite functional whose derivative with respect to the time variable is zero due to the energy preservation. As a consequence, the free energy functional $E(t)+|\varepsilon_L|$ is a Liapunov functional (see ref. 14 for a related Liapunov functional in this context) and the Lieb stationary solution is stable under small perturbations of the initial data in H^1 with respect to the minimal energy solution ψ_L. Also note that the asymptotic stability is not possible in this case due to the energy preservation.

5.1. Linear stability

The aim of this paragraph is to reinforce the previous result of stability by proving the linear stability for which we will first analyze the sign of the relative frequencies of oscillations through the expansion of the Action functional near the Lieb stationary solution. The analysis below rules out the possibility of having damped oscillations, i.e. eigenfrequencies not being neither purely real (stable motion) nor purely imaginary (unstable motion). We do not consider $1+3+3+3=10$ zero frequency modes here, associated with the broken symmetries of the stationary solution, namely, phase, translational, rotational and Galilean invariance. They do

not correspond to intrinsic deformations of the stationary solution, but rather to global transformations.

Let us study the stability of stationary solutions under " small" (non-zero mode) perturbations with respect to $\eta(x, t)$ of type

$$\psi(x, t) = e^{-i\varepsilon_L t}[\psi_L(x) + \eta(x, t)]. \tag{50}$$

Then, the idea is to expand $\mathscr{S}$ in the form

$$\mathscr{S}(\psi_L + \eta) = \mathscr{S}(\psi_L) + \mathscr{S}'(\psi_L)\,\eta + \tfrac{1}{2}\,\mathscr{S}''(\psi_L)(\eta, \eta) + \cdots \tag{51}$$

Since the Lieb solution ψ_L is a stationary solution to the SPS, then the linear term in an expansion of $\mathscr{S}$ around ψ_L is zero. Let us calculate the second order term. The second variation of the Action functional $\mathscr{S}$ is given by

$$\begin{aligned}\mathscr{S}''(\psi_L)(\eta, \eta) = \int_0^\infty \int_{\mathbb{R}^3} \bar{\eta}(x, t) \Bigg(& i\frac{\partial \eta}{\partial t}(x, t) + \varepsilon_L \eta(x, t) + \frac{1}{2m}\Delta_x \eta(x, t) \\ & - \frac{\gamma}{2\pi}\int_{\mathbb{R}^3} \frac{|\psi_L(x')|^2}{|x - x'|}\,dx'\,\eta(x, t))\,dx\,dt \\ & - \frac{\gamma}{8\pi}\int_0^\infty \frac{1}{|x - x'|}\,2\mathrm{Re}(\psi_L(x)\,\bar{\eta}(x, t)) \\ & \times 2\mathrm{Re}(\psi_L(x')\,\bar{\eta}(x', t))\,dx'\,dx\,dt.\end{aligned}$$

The function $\eta(x, t)$ is in general a complex function, and we may split it into real and imaginary parts as follows

$$\eta(x, t) = \mathrm{Re}\,\eta(x, t) + i\,\mathrm{Im}\,\eta(x, t) \equiv \eta_R(x, t) + i\eta_I(x, t). \tag{52}$$

To analyze the linear stability problem, the fact that the Lieb solution provides a global minimum of the energy functional for *real* functions proves essential. Note that our definition of energy, given in Lemma 2.1, is slightly different since it holds for *complex* functions but it obviously reduces to the real function case. All we want to prove in the following paragraph is that if the functional for real functions is minimized by ψ_L the functional for complex functions is also minimized by the same ψ_L. Indeed, Lieb's result $E[\psi]/\|\psi\|_{L_2} \geqslant E[\psi_L]/\|\psi_L\|_{L_2} \geqslant \varepsilon_L$ for any real $\psi(x)$ implies in particular that for any purely real perturbation $\eta_R(x)$ not being a zero mode, one has $E[\psi_L + \eta_R]/\|\psi_L + \eta_R\|_{L_2} > \varepsilon_L$. In the limit of small perturbation one gets that the second variation of the energy functional or, equiv-

alently, the associated quadratic form which we label by the operator $\mathscr{A}$ (defined below) is strictly larger than $\varepsilon_L \|\eta_R\|_{L_2}$, namely

$$\begin{aligned}\frac{1}{2}E''(\psi_L)(\eta_R,\eta_R) &\equiv \frac{1}{2}\langle \eta_R, \mathscr{A}\eta_R\rangle \\ &= \frac{1}{2m}\int_{\mathbb{R}^3}(\nabla\eta_R)^2\,dx - \frac{\gamma}{4\pi}\int_{\mathbb{R}^3}\frac{\psi_L(x')^2\,\eta_R(x)^2}{|x-x'|}\,dx' \\ &\quad -\frac{\gamma}{2\pi}\int_{\mathbb{R}^6}\frac{\psi_L(x)\,\eta_R(x)\,\psi_L(x')\,\eta_R(x')}{|x-x'|}\,dx'\,dx \\ &> \varepsilon_L\int_{\mathbb{R}^3}\eta_R(x)^2\,dx\end{aligned}$$

for all η_R. On the other hand, the second variation of the energy corresponding to a purely imaginary function $i\eta_I(x)$, which quadratic form is labeled by the operator $\mathscr{B}$ (defined below) fulfills

$$\begin{aligned}\frac{1}{2}E''(\psi_L)(\eta_I,\eta_I) &\equiv \langle \eta_I, \mathscr{B}\eta_I\rangle = \frac{1}{2m}\int_{\mathbb{R}^3}(\nabla\eta_I)^2\,dx - \frac{\gamma}{4\pi}\int_{\mathbb{R}^3}\frac{\psi_L(x')^2\,\eta_I(x)^2}{|x-x'|}\,dx' \\ &> \varepsilon_L\int_{\mathbb{R}^3}\eta_I(x)^2\,dx\end{aligned}$$

since $\mathscr{A}-\varepsilon_L$ is positive definite and $\mathscr{B}-\mathscr{A}$ is positive (in the attractive case) as can be deduced by considering the real function $\phi(x)\equiv\psi_L(x)\,\eta_R(x)$ and the convolution formula for the Coulomb energy functional

$$\int_{\mathbb{R}^6}\frac{\phi(x)\,\phi(x')}{|x-x'|}\,dx\,dx' = -\frac{1}{2\pi^2}\int_{\mathbb{R}^3}\frac{|\Phi(p)|^2}{p^2}\,dp < 0,$$

where $\Phi(p)=\bar{\Phi}(-p)=\int_{\mathbb{R}^3} e^{ip\cdot x}\,dx\,\phi(x)$ is the Fourier transformation of $\phi(x)$. Taking $\eta=\eta_R+i\eta_I$ both results combined imply that the second variation of the energy functional for *complex* variations fulfills

$$\begin{aligned}\frac{1}{2}E''(\psi_L)(\eta,\eta) &\equiv \frac{1}{2}\langle \eta, \mathscr{A}\eta\rangle \\ &= \int_{\mathbb{R}^3}\frac{1}{2m}|\nabla\eta(x)|^2\,dx - \frac{\gamma}{4\pi}\int_{\mathbb{R}^6}\frac{|\psi_L(x')|^2\,|\eta(x)|^2}{|x-x'|}\,dx'\,dx \\ &\quad +\frac{\gamma}{8\pi}\int_{\mathbb{R}^6}\frac{1}{|x-x'|}\,2\,\mathrm{Re}(\psi_L(x)\,\bar{\eta}(x,t)) \\ &\quad \times 2\mathrm{Re}(\psi_L(x')\,\bar{\eta}(x',t))\,dx'\,dx \\ &= \frac{1}{2}(E''(\psi_L(\eta_I,\eta_I)+E''(\psi_L(\eta_R,\eta_R)) > \varepsilon_L\int_{\mathbb{R}^3}|\eta(x)|^2\,dx,\end{aligned}$$

where we have denoted the complex extension of the operator $\mathscr{A}$ by the same symbol. Moreover, the second variation of the Action functional can be expressed in terms of the second variation of the energy functional as follows

$$\mathscr{S}''(\psi_L)(\eta, \eta) = \int_0^\infty \int_{\mathbb{R}^3} \bar{\eta}(x, t) \left(i \frac{\partial \eta}{\partial t}(x, t) + \varepsilon_L \eta(x, t) \right) dt - \int_0^\infty \langle \eta, \mathscr{A}\eta \rangle \, dt.$$

If we minimize this second variation with respect to the perturbation $\eta(x, t)$ and its complex conjugate $\bar{\eta}(x, t)$ independently we obtain the linear stability equations for $\bar{\eta}(x, t)$ and $\eta(x, t)$ respectively. In operator notation, the latter equation reads

$$i \frac{\partial n}{\partial t} + \varepsilon_L \eta = \mathscr{A}\eta$$

for the complex η. Expressing this function into real and imaginary parts, $\eta = \eta_R + i\eta_I$, this equation splits into two real equations,

$$\frac{\partial \eta_R}{\partial t} + \varepsilon_L \eta_I = \mathscr{B}\eta_I,$$

$$-\frac{\partial \eta_I}{\partial t} + \varepsilon_L \eta_R = \mathscr{A}\eta_R.$$

To solve the time dependence of this equation, let us propose as a solution the harmonic ansatz

$$\eta_R(x, t) = \alpha(x)\, e^{-i\omega t} + \bar{\alpha}(x)\, e^{i\bar{\omega}t}, \qquad \eta_I(x, t) = \beta(x)\, e^{-i\omega t} + \bar{\beta}(x)\, e^{i\bar{\omega}t}$$

yielding, in an obvious operator notation,

$$i\omega\beta = (\mathscr{A} - \varepsilon_L)\, \alpha, \qquad -i\omega\alpha = (\mathscr{B} - \varepsilon_L)\, \beta \tag{53}$$

which corresponds to a generalized eigenvalue problem for the vector-function (α, β). Since the operators $\mathscr{A} - \varepsilon_L$ and $\mathscr{B} - \varepsilon_L$ are hermitian and positive definite we can combine the equations (53) to obtain

$$\omega^2 \langle \alpha, (\mathscr{B} - \varepsilon_L)^{-1}\, \alpha \rangle = \langle \alpha, (\mathscr{A} - \varepsilon_L)\, \alpha \rangle \tag{54}$$

which gives $\omega^2 > 0$ and, hence, ω is real. Note that $\mathscr{B} - \varepsilon_L$ is in general an unbounded operator. However, in the context of H^1 solutions preserving energy the operator becomes bounded and (54) makes sense for the generalized eigen-solutions of (53).

Then, we have proved the following result:

Theorem 5.2. The solutions of the SPS which are small perturbations except for those associated with broken symmetries of the stationary solution, namely, phase, translational, rotational and Galilean invariance, of the stationary Lieb solution are linearly stable in the topology of L^∞.

6. EXISTENCE OF BREATHERS IN THE ATTRACTIVE CASE WITH NEGATIVE ENERGY

In this Section we will prove for negative energy the existence near the Lieb minimal solution of a bifurcation branch of periodic solutions (breathing modes). If we look for periodic solutions to the Schrödinger–Poisson problem, the natural constraint appears making the change of variables $t = \lambda s$ in the Schrödinger equation which can be then written as

$$i\lambda \frac{\partial \psi}{\partial s} = -\frac{1}{2m} \Delta\psi + V\psi \tag{55}$$

Then, seeking for 2π periodic solution in s correspond to $2\pi\lambda$ solutions in t. In this way λ measures the periodicity of the solutions to the system.

Consider the isoperimetric variational problem consisting in minimizing the energy functional

$$E = \int_0^{2\pi} \int_{\mathbb{R}^3} \left(\frac{1}{2m} |\nabla\psi(x, s)|^2 - \left(\int_{\mathbb{R}^3} \frac{|\psi(x', s)|^2}{4\pi\,|x - x'|}\, dx' \right) |\psi(x, s)|^2 \right) dx\, ds \tag{56}$$

over the constraints

$$\Sigma = \left\{ \int_0^{2\pi} \int_{\mathbb{R}^3} \left(\frac{i}{2} \left(\bar{\psi} \frac{\partial \psi}{\partial s} - \psi \frac{\partial \bar{\psi}}{\partial s} \right) + \frac{1}{2m} |\nabla\psi(x, s)|^2 \right.\right.$$
$$\left. - \left(\int_{\mathbb{R}^3} \frac{|\psi(x', s)|^2}{8\pi\,|x - x'|}\, dx' \right) |\psi(x, s)|^2 \right) dx\, ds = \frac{8}{3}\pi(\varepsilon_L + R),\ 0 < R < |\varepsilon_L|;$$
$$\left. \int_0^{2\pi} (-\Delta\psi\bar{\psi} + \Delta\bar{\psi}\psi)\, ds = 0 \right\}. \tag{57}$$

The idea is that in this variational principle the period λ appear as a Lagrange multiplier and the possible solutions of the isoperimetric varia-

tional system lead to a non-constant periodic solution which has eigenvalue $\varepsilon_L + R$, with $R > 0$. The solutions will belong to a subspace of the Sobolev space $H^1(0, 2\pi; H^2(\mathbb{R}^3))$ of 2π periodic functions. The possible periodicity will appear on the density function and not over the wave function via the continuity equation

$$i\lambda \frac{\partial |\psi|^2}{\partial s} = \frac{1}{2m} (-\Delta\psi\bar{\psi} + \Delta\bar{\psi}\psi).$$

Let us first see that the second constraint, which gives the periodicity of the density, does not affect to the form of the associated Euler–Lagrange equation.

Lemma 6.8. The constraint

$$\int_0^{2\pi} (-\Delta\psi\bar{\psi} + \Delta\bar{\psi}\psi)\, ds = 0 \tag{58}$$

does not contribute with any tern to the Euler–Lagrange equation associated to the isoperimetric variational problem which has the form (55).

Proof. The Lagrange multiplier associated to the constraint (58) depends on x and provides the following term in the extended functional associated to the isoperimetric problem (56)–(57)

$$\int_0^{2\pi} \int_{\mathbb{R}^3} \beta(x)(-\Delta\psi\bar{\psi} + \Delta\bar{\psi}\psi)(x, s)\, dx\, ds$$

which can be written after integrating by parts as follows

$$\int_0^{2\pi} \int_{\mathbb{R}^3} \nabla\beta(x)\, Q(x, s)\, dx\, ds, \tag{59}$$

where

$$Q(x, s) = (\nabla\psi\bar{\psi} - \nabla\bar{\psi}\psi)(x, s). \tag{60}$$

On the other hand, the variation of the isoperimetric variational problem with respect to $\bar{\psi}$ and with respect to ψ provides the equations

$$i\lambda \frac{\partial\psi}{\partial s} = -\frac{1}{2m} \Delta\psi + V\psi + \beta\, \Delta\psi - \Delta(\beta\psi) \tag{61}$$

$$-i\lambda \frac{\partial\bar{\psi}}{\partial s} = -\frac{1}{2m} \Delta\bar{\psi} + V\bar{\psi} - \beta\, \Delta\bar{\psi} + \Delta(\beta\bar{\psi}). \tag{62}$$

Then, multiplying the first equation by $\bar{\psi}$ and the second one by ψ and adding them we have

$$i\lambda \frac{\partial |\psi|^2}{\partial s} = \frac{1}{2m}(-\Delta\psi\bar{\psi} + \Delta\bar{\psi}\psi) - 2\nabla\beta\,\nabla|\psi|^2 - 2\Delta\beta\,|\psi|^2.$$

Now, integrating over $(0, 2\pi)\times\mathbb{R}^3$ and taking into account the constraints we find

$$0 = \int_0^{2\pi}\int_{\mathbb{R}^3} (\nabla\beta^2\,\nabla|\psi|^2 + 2\Delta\beta\beta\,|\psi|^2)\,dx\,ds = -\int_0^{2\pi}\int_{\mathbb{R}^3} |\nabla\beta|^2\,|\psi|^2\,dx\,ds,$$

which implies that $\nabla\beta = 0$ and, therefore, the term (59) in the extended functional associated to the isoperimetric problem does not contribute to the corresponding Euler–Lagrange equation that takes the form (55).

Lemma 6.9. The Lagrange multipliers λ and α associated with the first constant in Sigma ans with $\|\psi\|_{L^2} \leqslant 1$ satisfy

$$\left(\frac{4}{3}(\varepsilon_L + R) - \frac{1}{2\pi}\int_0^{2\pi} E(s)\,ds\right)\lambda = \frac{1-\lambda}{2\pi}\int_0^{2\pi} Q(s)\,ds - \alpha\,\|\psi\|_{L^2}, \tag{63}$$

where

$$Q = \int_{\mathbb{R}^3}\left(\frac{1}{2m}|\nabla\psi|^2 + V\,|\psi|^2\right)dx. \tag{64}$$

Proof. From the Euler–Lagrange equations associated to ψ and $\bar{\psi}$ we obtain

$$i\lambda\left(\frac{\partial\psi}{\partial s}\bar{\psi} - \frac{\partial\bar{\psi}}{\partial s}\psi\right) + 2\alpha\,|\psi|^2 = (1-\lambda)\left(-\frac{1}{m}(\Delta\psi\bar{\psi} + \Delta\bar{\psi}\psi) + 2V\,|\psi|^2\right).$$

Integrating by parts over $(0, 2\pi)\times\mathbb{R}^3$ we deduce

$$i\lambda\int_0^{2\pi}\int_{\mathbb{R}^3}\left(\frac{\partial\psi}{\partial s}\bar{\psi} - \frac{\partial\bar{\psi}}{\partial s}\psi\right)dx\,ds + 4\pi\alpha\,\|\psi\|^2_{L^2(\mathbb{R}^3)} = 2(1-\lambda)\int_0^{2\pi} Q(s)\,ds,$$

from which we have the result. ∎

Denote by H the closed convex set belongs to the Hilbert space $H^1(0, 2\pi; H^2(\mathbb{R}^3))$:

$$H = \{\psi \in H^1(0, 2\pi; H^2(\mathbb{R}^3)) \text{ such that } \|\psi\|_{L^2} \leqslant 1\}.$$

Lemma 6.10. Let $\psi \in H^1(0, 2\pi; H^2(\mathbb{R}^3))$ such that $\|\psi\|_{L^2} \leqslant 1$ and such that ψ is a minimum of (56). Then, $\|\psi\|_{L^2} = 1$.

Proof. The proof consists in assuming that $\|\psi\|_{L^2} = \sigma < 1$ and letting $\phi = \sigma^{-1}\psi$. Then, it is easy to deduce that $E(\phi) < \sigma^{-2}E(\psi)$ in contradiction with the fact that ψ is the minimum of (56). ∎

We now investigate the functionals that define the set Σ.

Lemma 6.11. The defining functionals of Σ are continuous with respect to the weak convergence in H.

Proof. Let $\{\psi_j\}$ be a sequence weakly convergent to ψ in H. Then, writing

$$\frac{i}{2}\int_0^{2\pi}\int_{\mathbb{R}^3}\left(\left\{\bar{\psi}_j\frac{\partial\psi_j}{\partial s}-\psi_j\frac{\partial\bar{\psi}_j}{\partial s}\right\}-\left\{\bar{\psi}\frac{\partial\psi}{\partial s}-\psi\frac{\partial\bar{\psi}}{\partial s}\right\}\right)dx\,ds$$

$$=\frac{i}{2}\int_0^{2\pi}\int_{\mathbb{R}^3}\left\{(\bar{\psi}_j-\bar{\psi})\frac{\partial\psi_j}{\partial s}+\bar{\psi}\left(\frac{\partial\psi_j}{\partial s}-\frac{\partial\psi}{\partial s}\right)\right.$$

$$\left.+\psi\left(\frac{\partial\bar{\psi}}{\partial s}-\frac{\partial\bar{\psi}_j}{\partial s}\right)+(\psi-\psi_j)\frac{\partial\bar{\psi}_j}{\partial s}\right\}dx\,ds$$

and taking into account the duality in L^2, we deduce the required continuity for the first functional in Σ. Note that we have strongly used the convergence of the terms involving in the quadratic expressions by means of the compactness of Sobolev embedding on compact domains. Similarly, for the second constraint in Σ we operate in a weak formulation in the space variable for the functional

$$\int_0^{2\pi}\int_{\mathbb{R}^3}(-\Delta\psi\bar{\psi}+\Delta\bar{\psi}\psi)\,\Phi\,dx\,ds, \qquad \forall\Phi\in C_0^\infty(\mathbb{R}^3). \quad ∎$$

In order to prove that the isoperimetric problem has a minimum, let us introduce some necessary tools. Consider the space of the symmetric decreasing functions

$$S=\{f:\mathbb{R}^3\to[0,\infty] \text{ such that } f(x)\leqslant f(y) \text{ if } |x|\geqslant|y|\}$$

and let

$$S'=\{f:\mathbb{R}^3\to[0,\infty] \text{ such that } f(x-v)=g(x) \text{ a.e.}$$
$$\text{for some } v\in\mathbb{R}^3 \text{ and } g\in S\}$$

be the translates a.e of functions in S. If χ is the characteristic function of a measurable set in $\mathbb{R}^3$, χ will denote

$$\chi(x)=\begin{cases}1 & \text{if} \quad 4\pi\,|x|^3/3 \leqslant \|\chi\|_{L^1}\\ 0 & \text{otherwise.}\end{cases}$$

Clearly $\chi^* \in S$ and $\|\chi\|_{L^1}=\|\chi^*\|_{L^1}$. Given $f\colon \mathbb{R}^3 \to [0, \infty]$, let $\chi_a^f(x)=1$ if $f(x) \geqslant a$, $\chi_a^f(x)=0$ otherwise. Then $f(x)=\int_0^\infty \chi_a^f(x)\,da$, and we define its decreasing rearrangement

$$f^*(x) \stackrel{def}{=} \int_0^\infty (\chi_a^f)^*(x)\,da. \tag{65}$$

Clearly $f^* \in S$ and is equimeasurable with f.

In our context, let us first note that a solution of the isoperimetric variational problem (56)–(57) is invariant under change of phase of type $e^{-i2\pi(\varepsilon_L+R)t}\psi(t, x)$. Then, it will be important that our minimizing solution verifies this property. Also, we will deal with time-depending complex valuated functions which requires the following definition of symmetric decreasing rearrangement of $\psi\colon \mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{C}$

$$\psi^* \stackrel{def}{=} |\psi|^*, \tag{66}$$

where the rearrangement is taken in the space variable for every $t \in \mathbb{R}^+$ fixed, and it is defined except for a multiplier change of phase $e^{-i2\pi(\varepsilon_L+R)t}$ on ψ. Then, we define the space

$$S_{\varepsilon_L+R}=\{e^{-i(\varepsilon_L+R)t}\psi(t, x), \text{ with } \psi \in H \cap S\}, \tag{67}$$

where $e^{-i(\varepsilon_L+R)t}\,|\psi(t, x)|^*$ belongs.

The next result relates the energy of a wave function ψ with those of its rearrangement ψ^*. The proof is based on the properties of the symmetric decreasing rearrangement functions and on the Riesz inequality, see ref. 16.

Lemma 6.12. Assume that $\psi \in L^\infty(0, \infty; H^1(\mathbb{R}^3))$. Then, the following assertions are verified

1. If $|\psi| \notin S'$, then

$$\int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3}\frac{|\psi(x', s)|^2}{4\pi\,|x-x'|}\,dx'\right)|\psi(x, s)|^2\,dx$$
$$<\int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3}\frac{|\psi(x', s)|^2}{4\pi\,|x-x'|}\,dx'\right)|\psi(x, s)|^2\,dx. \tag{68}$$

2. If $\psi(\cdot, s) \in H^2(\mathbb{R}^3)$, then $\psi(\cdot, s) \in H^2(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} |\nabla \psi(x, s)|^2 \, dx \geqslant \int_{\mathbb{R}^3} |\nabla \psi^*(x, s)|^2 \, dx. \tag{69}$$

Let us now establish the existence of a minimizing sequence of symmetric decreasing rearrangement wave functions. To do that, let us consider the extended energy functional

$$\tilde{E} = \int_0^{2\pi} \int_{\mathbb{R}^3} \left\{ \left(\frac{1}{2m} |\nabla \psi(x, s)|^2 - \left(\int_{\mathbb{R}^3} \frac{|\psi(x', s)|^2}{4\pi |x - x'|} \, dx' \right) |\psi(x, s)|^2 \right) - \lambda \frac{i}{2} \left(\bar{\psi} \frac{\partial \psi}{\partial s} - \psi \frac{\partial \bar{\psi}}{\partial s} \right) - \beta(x)(-\Delta \psi \bar{\psi} + \Delta \bar{\psi} \psi) \right\} dx \, ds. \tag{70}$$

Lemma 6.13. i) There exists a minimizing sequence of symmetric decreasing functions $\{\psi_j\}_{j \in \mathbb{N}} \subset S_{\varepsilon_L + R}$ for $\tilde{E}$.

ii) If $\psi \in S_{\varepsilon_L + R}$ is a solution of the isoperimetric variational problem, then $\psi \in S'$.

Proof. Let $\{\psi_j\}_{j \in \mathbb{N}} \subset H$ a minimizing sequence for the isoperimetric problem. To deduce i), we replace ψ_j by ψ_j^*, use Lemmas 6.10 and 6.12, the equality $\|\psi_j(\cdot, s)\|_{L^2} = \|\psi_j^*(\cdot, s)\|_{L^2}$ and the fact that ψ_j is a real function except for a phase factor of type $e^{-i(\varepsilon_L + R)s}$ which implies that the two last terms in $\tilde{E}$ are zero to an additive term for the first one which is $\pi(\varepsilon_L + R)$ in agreement with the first constraint in Σ.

ii) follows from the first part of Lemma 6.12. ∎

The following Lemma gives us the necessary a priori estimates to deal with the minimizing sequence.

Lemma 6.14. The functions ψ that minimize the functional E are at least $H^1(\mathbb{R}^3)$ functions for every $t \in \mathbb{R}^+$.

Proof. It is a direct consequence of the facts that the energy is finite and bounded from below by the energy associated to the Lieb minimal solution and that the potential energy can be bounded in terms of the

kinetic energy (as it has been obtained in an optimal way for the attractive case in Section 6) for example by using the bounds

$$\int_{\mathbb{R}^3} \left(\int_{\mathbb{R}^3} \frac{|\psi(x', s)|^2}{4\pi\, |x-x'|}\, dx' \right) |\psi(x, s)|^2\, dx$$

$$\leqslant \|n(\cdot, t)\|_{L^1(\mathbb{R}^3)} \left(c_{M_1} \|n(\cdot, t)\|_{L^1(\mathbb{R}^3)} + c_{M_2} \|n(\cdot, t)\|_{L^3(\mathbb{R}^3)}\right)$$

$$\leqslant \|n(\cdot, t)\|_{L^1(\mathbb{R}^3)} \left(c_{M_1} \|n(\cdot, t)\|_{L^1(\mathbb{R}^3)} + c_s c_{M_2} \|\nabla\psi(\cdot, t)\|_{L^2(\mathbb{R}^3)}\right),$$

where c_{M_1} and c_{M_2} are constants depending on the integral of the kernel $|x|^{-1}$ inside and outside the ball of center 0 and radius M respectively, and c_s is the Sobolev constant associated to the injection $H^1 \subset L^6$ in $\mathbb{R}^3$. Then, we can choose M such that $c_S c_{M^2} < 1$ which leads to the announced bound. ∎

We now give the proof of the existence of a minimum in $S_{\varepsilon_{L+R}}$ which is basically a consequence of the previous Lemmas and of the Lieb ideas[16].

Theorem 6.3. The isoperimetric variational problem has a solution in $S_{\varepsilon_{L+R}}$.

Proof. Let $\psi_j \in S_{\varepsilon_{L+R}}$ be a minimizing sequence for the isoperimetric variational problem constructed as in Lemma 6.13. By Lemma 6.14 $\|\nabla\psi_j(\cdot, s)\|_{L^2}$ is bounded from which we deduce by the Banach–Alaoglu theorem the existence of a H^1-weakly convergent subsequence. If ψ is the weak limit then

$$\|\psi\|_{L^2} \leqslant 1 \qquad \text{and} \qquad \liminf_{j\to\infty} \int_{\mathbb{R}^3} |\nabla\psi_j(x, s)|^2\, dx \geqslant \int_{\mathbb{R}^3} |\nabla\psi(x, s)|^2\, dx.$$

Let $n_j(x, s) = |\psi_j(x, s)|^2 \in S$. We will also denote by $n(|x|, s)$ the density for spherically symmetric functions. By Lemma 6.14 $n_j(x, s) \in L^3(\mathbb{R}^3)$. Then, for any $M \geqslant 0$ we have

$$n_j(M, s)\, 4\pi M^3/3 \leqslant 4\pi \int_0^M n_j(\sigma, s)\, \sigma^2\, d\sigma \leqslant \|n_j(\cdot, s)\|_{L^1(\mathbb{R}^3)} \leqslant 1$$

$$n_j^3(M, s)\, 4\pi M^3/3 \leqslant C.$$

Thus $n_j(M, s) < f(M)$ for $s \in \mathbb{R}^+$, where $f(r) = Ar^{-1}$, for $r \leqslant 1$ and $f(r) = Ar^{-3}$, for $r \geqslant 1$, and A is an upper bound of the previous constants.

We also have a uniform L^1 estimate of the gradients of the density which is again a consequence of the boundedness of $\nabla\psi_j(\cdot, s)$ in $L^2(\mathbb{R}^3)$.

Then, as a consequence of the Helly theorem, we can deduce that $n_j(r, s) \to n(r, s) \leqslant f(r)$ point-wise for $r > 0$. We deduce that $n = |\psi|^2$ by using that $\psi_j \to \psi$ weak in L^2 and $|\psi_j| \leqslant f^{1/2} \in L^2_{loc}$.

Since $n_j \to n = |\psi|^2$ point-wise, and $n \leqslant f$, the dominated convergence theorem assure us that

$$\int_{\mathbb{R}^6} \frac{|\psi_j(x', s)|^2}{4\pi |x - x'|} |\psi_j(x, s)|^2 \, d(x', x) \to \int_{\mathbb{R}^6} \frac{|\psi(x', s)|^2}{4\pi |x - x'|} |\psi(x, s)|^2 \, d(x', x)$$

provided that

$$\int_{\mathbb{R}^3} \left(\int_{\mathbb{R}^3} \frac{f(|x'|)}{4\pi |x - x'|} \, dx' \right) f(|x|) \, dx < \infty.$$

Combining the above estimates we have $E = \liminf_{j \to \infty} E(\psi_j) \geqslant E(\psi)$. Hence, ψ is a minimum for E. ∎

Let us now analyze some properties of the minimizing function ψ.

Theorem 6.4. 1. If $\psi \in H$ is an infimum of the isoperimetric variational problem, then ψ satisfies

$$i\lambda \frac{\partial \psi}{\partial s} = -\frac{1}{2m} \Delta \psi + V\psi, \tag{71}$$

$$\Delta V = |\psi|^2. \tag{72}$$

2. The solution of the isoperimetric problem given in Theorem 6.3 takes the form $e^{-i(\varepsilon_L + R)s} \psi(x)$, with $\psi \in S$ and verifies

$$(\varepsilon_L + R)\, \psi = -\frac{1}{2m} \Delta \psi + V\psi. \tag{73}$$

Proof. The first assertion is a consequence of the fact that the minimum of the isoperimetric variational problem (56)–(57) verifies the associated Euler–Lagrange equation.

The second assertion can be deduced from the fact that the solution constructed in Theorem 6.3 must be of the type $e^{-i(\varepsilon_L + R)s} \psi(x, s)$, where $\psi(x, s) \in S$ verifies

$$(\lambda(\varepsilon_L + R) + \alpha)\, \psi = (1 - \lambda) \left(-\frac{1}{2m} \Delta \psi + V\psi \right) - i\lambda \frac{\partial \psi}{\partial s}. \tag{74}$$

from this equation we deduce (multiplying by $\bar{\psi}$) that ψ does not depend on t. Using now the first assertion of this theorem and (63)–(64) we obtain

$$Q\psi = -\frac{1}{2m}\Delta\psi + V\psi.$$

From the relation between Q and E, $Q = 3E$, we deduce taht $Q = \varepsilon_L + R$. Finally, since $\varepsilon_L + R < 0$, then $\psi \in C^\infty(\mathbb{R}^3)$ and goes to zero at infinity (see ref. 16), and hence $e^{-i(\varepsilon_L + R)s}\psi(x)$ is a classical solution of (74). ▌

The above Lemmas allow to establish the following result.

Theorem 6.5. In the attractive case with negative energy there exists a unaparametric ($0 < R < |\varepsilon_L|$) bifurcation branch of periodic solutions (breathing modes) from the Lieb solution.

Remark. On the commensurability condition for periodic solutions and the relevance of Theorem 6.5: In classical mechanics it is well known (Poincaré's theorem) that a sufficient condition for a Hamiltonian system to preserve periodic motion under small nonlinear perturbations of the initial data is that the frequencies of the unperturbed system be incommensurable, i.e. their ratios should not be integer numbers. This condition is actually not necessary for a restricted class of perturbations and in particular to purely perturbed initial data without changing the Hamiltonian functional (see ref. 2), but it may nevertheless be verified in a system with a finite number of degrees of freedom. Thus, one can use the Poincaré theorem to prove, but not to disprove periodic motion under small perturbations. For a system with "infinite" degrees of freedom, like a partial differential equation, the commensurability condition may actually be difficult to check, since one is searching for a very specific spectral information on a quadratic form defined on a Hilbert space. Actually, if the quadratic form turns out to have a continuous spectrum it is most likely that the incommensurability condition is not met. The strength of our Theorem 6.5 is that due to convexification properties, through the rearrangement, of the energy functional it is really not necessary to analyze the spectrum of the second variation around the Lieb's solution.

ACKNOWLEDGMENTS

The authors thanks L. L. Bonilla for calling our attention on the commensurability condition for periodic solutions in relation with our result in Section 6. This work was partially supported by DGES (Spain),

Projects PB98-1281 and PB98-1367 and by European Union-TMR, contract ERB FMBX-CT97-0157.

REFERENCES

1. P. Bechouche, J. Nieto, E. Ruiz Arriola, and J. Soler, On the time evolution of the mean-field polaron, *J. Math. Phys.* **41**:4293–4312 (2000).
2. M. S. Berger, *Nonlinearity and Functional Analysis* (Academic Press, New York, 1977).
3. F. Brezzi and P. A. Markowich, The three-dimensional Wagner–Poisson problem: existence, uniqueness and approximation, *Math. Mod. Meth. Appl. Sci.* **14**:35–61 (1991).
4. F. Castella, L^2-solutions to the Schrödinger–Poisson system: existence, uniqueness, time behaviour and smoothing effects, *Math. Mod. Meth. Appl. Sci.* **7**:1051–1083 (1997).
5. H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon, Schrödinger operators with application to quantum mechanics and global geometry, *Texts and Monographs in Physics* (Springer-Verlag, 1987).
6. J. Christian, An exactly soluble sector of quantum gravity, *Physical Review D* **56**:4844 (1997).
7. R. T. Glassey, Asymptotic behaviour of solutions to certain nonlinear Schrödinger–Hartree equations, *Commun. Math. Phys.* **53**:9–18 (1977).
8. H. Goldstein, *Classical Mechanics*, Second Ed. (Addison Wesley, 1980).
9. E. L. HILL, Hamilton's principle and the conservation theorems of mathematical physics, *Rev. Mod. Phys.* **23**:253–260 (1951).
10. R. Illner, P. F. Zweifel, and H. Lange, Global existence, uniqueness and asymptotic behaviour of solutions of the Wigner–Poisson and Schrödinger–Poisson systems, *Math. Meth. Appl. Sci.* **17**:349–376 (1994).
11. K. R. W. Jones, Newtonian quantum gravity, *Austral. J. Phys.* **48**:1055 (1995).
12. D. Kumar and V. Soni, Single Particle Schrödinger equation with Gravitational self-interaction, *Phys. Lett. A* **271**:157 (2000).
13. L. D. Landau, and E. M. Lifshitz, *Theoretical Physics*, Part 1, 3rd. ed. (Pergamon P., Oxford, 1980).
14. H. Lange, and P. F. Zweifel, Dissipation in Wigner- -Poisson systems, *J. Math. Phys.* **35**:1515–1521 (1995).
15. J. M. Levy-Leblond, Galilei group and nonrelativistic Quantum Mechanics, *J. Math. Phys.* **4**:776–788 (1963).
16. E. H. Lieb, Existence and uniqueness of the minimizing solution of Choquard's nonlinear equation, *Studies in Appl. Math.* **57**:93–105 (1977).
17. P. L. Lions and T. Paul, Sur les mesures de Wigner, *Revista Matemática Iberoamericana* **9**553–618 (1993).
18. J. L. López and J. Soler, Scaling limits in the 3-D Schrödinger–Poisson system, *Appl. Math. Lett.* **10**:61-65 (1997).
19. J. L. López and J. Soler, Asymptotic behaviour to the 3-D Schrödinger/Hartree–Poisson and Wigner–Poisson systems, *Math. Mod. Meth. in App. Sci.* **10**:923–943 (2000).
20. P. A. Markowich, C. Ringhofer, and C. Schmeiser, *Semiconductor Equations* (Springer-Verlag, 1990).
21. S. Miyake, Strong coupling limit of the polaron ground state, *J. Phys. Soc. Jpn.* **38**:181 (1975).
22. I. M. Moroz, R. Penrose, and K. P. Tod, Spherically-symmetric solutions of the Schrödinger–Newton equations, *Class. Quantum Gravity* **15**:2733 (1998).

23. U. Niederer, The maximal kinematical invariance group of the free Schrödinger equation, *Helvetica Physica Acta*, **45**:802–810 (1972).
24. F. Nier, A variational formulation of Schrödinger–Poisson systems in dimension $d \leqslant 3$, *Comm. Part. Diff. Eq.* **18**:1125–1147 (1993).
25. E. C. G. Sudarshan and N. Mukunda, *Classical Mechanics: A Modern Perspective* (Wiley, 1974).
26. R. Penrose, On Gravity's Role in Quantum State Reduction, *Gen. Rel. and Grav.* **28**:581 (1996).
27. V. Soni, *Planck Scale Physics of the Single Particle Schrödinger Equation with Gravitational Self- Interaction*, Preprint September 2000, gr-qc/0009065.
28. P. Tod and I. M. Moroz, An analytical approach to the Schrödinger–Newton equation, *Nonlinearity* **12**:201 (1999).