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Existence and Nonlinear Stability of Stationary States of the Schrödinger–Poisson System

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We consider the Schrödinger–Poisson system in the repulsive (plasma physics) Coulomb case. Given a stationary state from a certain class we prove its nonlinear stability, using an appropriately defined energy-Casimir functional as Lyapunov function. To obtain such states we start with a given Casimir functional and construct a new functional which is in some sense dual to the corresponding energy-Casimir functional. This dual functional has a unique maximizer which is a stationary state of the Schrödinger–Poisson system and lies in the stability class. The stationary states are parameterized by the equation of state, giving the occupation probabilities of the quantum states as a strictly decreasing function of their energy levels.

KEY WORDS: Hartree problem; Schrödinger–Poisson system; stationary solutions; nonlinear stability.

1. INTRODUCTION

A large ensemble of charged quantum particles interacting only by the electrostatic field which they create collectively can be modelled by the Hartree problem:

$$i \frac{\partial R}{\partial t} = [H_V, R] \tag{1.1}$$

$$\triangle V = -n \tag{1.2}$$

$$n(t, x) = R(t, x, x) \tag{1.3}$$

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Here $R(t)$ denotes the density operator of the system, a time dependent, hermitian, positive trace class operator acting on the Hilbert space $L^2(\Omega)$, $\Omega \subset \mathbb{R}^3$ being the spatial domain in which the particles are confined. Equation (1.1) is the von Neumann–Heisenberg equation, where the potential V in the Hamiltonian $H_V := -\Delta + V(t, x)$ is given as the solution of the Poisson equation (1.2), subject to a homogeneous Dirichlet boundary condition

$$V(t, x) = 0, \qquad t \geqslant 0, \quad x \in \partial\Omega \tag{1.4}$$

By abuse of notation $R(t, x, y)$ denotes the L^2-kernel of the trace class operator $R(t)$, and its trace is the spatial charge density $n = n(t, x)$. The Hartee problem was rigorously derived as the weak-coupling mean field limit of a repulsively interacting particle ensemble by Spohn[25] under the assumptions of a bounded interaction potential and molecular chaos. Recently, the assumption on the potential was generalized, explicitely allowing the electrostatic Coloumb interaction.[4] We remark that the Hartree system does not take into account the Pauli exclusion principle, as opposed to the Hartree–Fock system, cf. refs. 8 and 12, which currently is under intensive scrutiny.

The Hartree picture is equivalent to the Schrödinger–Poisson picture, which is more suitable for our present purposes and is obtained as follows: Let (ϕ_k) be a complete orthonormal sequence of eigenvectors of $R(0)$ with eigenvalues (λ_k) and let $(\psi_k(t, \cdot))$ be the solution of the Schrödinger–Poisson system

$$i\,\frac{\partial \psi_k}{\partial t} = -\Delta\psi_k + V\psi_k \tag{1.5}$$

$$\Delta V = -n \tag{1.6}$$

$$n = \sum_{k=1}^{\infty} \lambda_k\, |\psi_k|^2 \tag{1.7}$$

with initial data $\psi_k(0) = \phi_k$. Then

$$R(t, x, y) = \sum_k \lambda_k \psi_k(t, x)\, \bar{\psi}_k(t, y) \tag{1.8}$$

defines the L^2-kernel of an operator $R(t)$ which solves the von Neumann–Heisenberg equation (1.1) with the corresponding initial datum, and vice versa. In the Schrödinger–Poisson picture $\psi_k = \psi_k(t, x)$ is the wave function of the kth state, $k \in \mathbb{N}$, $\lambda_k \geqslant 0$ denote the corresponding occupation probabilities normalized such that $\sum_k \lambda_k = 1$, $n = n(t, x)$ is the number density, and $V = V(t, x)$ is again the self-consistent potential of the ensemble. In order to avoid continuous spectra we shall analyze this system on a bounded domain $\Omega \subset \mathbb{R}^3$ with sufficiently smooth boundary, and we supplement it with Dirichlet boundary conditions:

$$\psi_k(t, x) = 0, \quad V(t, x) = 0, \quad t \geqslant 0, \quad x \in \partial\Omega, \quad k \in \mathbb{N} \tag{1.9}$$

We could also consider the system on the whole space $\mathbb{R}^3$ and add to V a confining exterior potential V_e, in which case the obtained results and their proofs need only minor modifications. Initial data are given by a complete orthonormal system $(\psi_k(\cdot, 0))$ in $L^2(\Omega)$. We refer to refs. 1, 5, 12, and 19 for background information on the Schrödinger–Poisson system (1.5), (1.6), (1.7).

The purpose of the present paper is to investigate the nonlinear stability of certain stationary states of the Schrödinger–Poisson system, i.e., of solutions of the form $\psi_k(t, x) = e^{i\mu_k t}\phi_k(x)$ with energy levels $\mu_k \in \mathbb{R}$, and we prove the existence of such stationary states. To our knowledge, the stability problem has not yet been investigated. The existence problem has been considered before by different methods and under various sets of assumptions, cf. refs. 19–22.

Our approach is motivated by analogous results for the Vlasov–Poisson system which arises as the classical limit of the Schrödinger–Poisson system. Both systems share the following property: The total energy of the system is conserved along solutions—indeed, the dynamics can be interpreted as the "Hamiltonian flow" induced by the energy functional—, but the stationary states are not critical points of the energy. On the other hand, there exist additional conserved quantities, the so-called Casimir functionals,[6] such that a given stationary state is a critical point for the appropriately chosen energy-plus-Casimir functional $\mathscr{H}_C$. The energy-Casimir method was first used to prove genuine, nonlinear stability for fluid-flow problems by Arnol'd in the 1960's, cf. refs. 2 and 3. Some of the background of this method can be found in ref. 18. More recently, the energy-Casimir method was adapted to problems in kinetic theory, in particular the Vlasov–Poisson system, cf. refs. 13–17, 23, 24, 26, and 27. When applying this method there is a sharp contrast between the plasma physics situation and the stellar dynamics one, where the sign in the Poisson equation is reversed: The quadratic part in the expansion of the energy-Casimir functional at the stationary state is positive definite in the plasma physics case while it is indefinite in the stellar dynamics case. Therefore, in the former case the method applies in a straight forward manner, cf. ref. 23, while in the latter case a careful investigation of the behavior of the energy-Casimir functional along minimizing sequences is needed and leads to non-linear stability only for such stationary states which are obtained as minimizers of this functional. The present paper addresses the plasma-physics case for the Schrödinger–Poisson system—certainly, the quantum-attractive case is mathematically more difficult but also physically less interesting—, and thus the approach should be more like the former case for the Vlasov–Poisson system.

This is indeed so: In Section 3 we show that stationary states (ψ_0, λ_0) from a specified class are nonlinearly stable. The proof relies on estimating the difference $\mathscr{H}_C(\psi, \lambda) - \mathscr{H}_C(\psi_0, \lambda_0)$ from below by an expression which is quadratic in $(\psi, \lambda) - (\psi_0, \lambda_0)$, where (ψ, λ) is some other, "close-by" state, and observing that the energy-Casimir functional $\mathscr{H}_C$ is constant along solutions of the Schrödinger–Poisson system. In Section 4 we construct a functional which is in some sense dual to a given energy-Casimir functional. This dual functional is known in the literature and has been used to construct stationary states, cf. ref. 21, but its relation to the energy-Casimir functional is to our knowledge new and should be useful for related problems. The dual functional turns out to be concave, and by variational techniques we show in Section 5 that it has a unique maximizer, which is a stationary state, and nonlinearly stable by Section 3. We emphasize that—as opposed to the stellar-dynamics situation for the Vlasov–Poisson system—the stability analysis and the existence analysis are independent from each other; the connecting Section 4 puts both parts into a common perspective. Before going into all this we introduce the class of stationary states and Casimir functionals under consideration, derive some preliminary estimates, and fix some notation.

2. PRELIMINARIES

As state space for the Schrödinger–Poisson system we use the set

$$\mathscr{S} := \Big\{ (\psi, \lambda) \mid \psi = (\psi_k)_{k\in\mathbb{N}} \subset H_0^1(\Omega) \cap H^2(\Omega)$$

$$\text{is a complete orthonormal system in } L^2(\Omega),$$

$$\lambda = (\lambda_k)_{k\in\mathbb{N}} \in l^1 \text{ with } \lambda_k \geqslant 0,\ k \in \mathbb{N},$$

$$\sum_k \lambda_k \int |\triangle\psi_k|^2 < \infty \Big\}$$

$\sum_k$ always means $\sum_{k=1}^{\infty}$. Our notation for the Sobolev spaces H^2 and H_0^1 is the standard one; by $\|\cdot\|_p$ we will denote the norm in the usual L^p space. For $(\psi, \lambda) \in \mathcal{S}$ we have

$$n_{\psi,\lambda} := \sum_k \lambda_k \, |\psi_k|^2 \in L^2(\Omega)$$

and $V_{\psi,\lambda}$ denotes the Coulomb potential induced by $n_{\psi,\lambda}$, i.e.,

$$\triangle V_{\psi,\lambda} = -n_{\psi,\lambda} \quad \text{on } \Omega, \qquad V_{\psi,\lambda} = 0 \quad \text{on } \partial\Omega$$

note that $V_{\psi,\lambda} \in H_0^1(\Omega) \cap H^2(\Omega)$ by the energy bound and Sobolev inequalities. For every initial state $(\psi(0), \lambda) \in \mathcal{S}$ there is a unique strong solution $[0, \infty[\, \ni t \mapsto \psi(t)$ of (1.5)–(1.9) with $(\psi(t), \lambda) \in \mathcal{S}$, cf. ref. 5. Throughout the paper, potentials V are real-valued while quantum states ψ_k are complex-valued. The energy of a state $(\psi, \lambda) \in \mathcal{S}$ is defined as

$$\begin{aligned}\mathcal{H}(\psi, \lambda) &:= \sum_k \lambda_k \int |\nabla \psi_k|^2 + \frac{1}{2} \int n_{\psi,\lambda} V_{\psi,\lambda} \\ &= \sum_k \lambda_k \int |\nabla \psi_k|^2 + \frac{1}{2} \int |\nabla V_{\psi,\lambda}|^2\end{aligned}$$

integrals always extend over the set Ω. The energy is conserved along solutions of the Schrödinger–Poisson system, indeed, the system (1.5)–(1.9) can be written in the form

$$\begin{aligned} i\,\frac{\partial \psi_k}{\partial t} &= -\frac{1}{2\lambda_k}\,\delta_{\bar{\psi}_k} \mathcal{H}, \\ i\,\frac{\partial \bar{\psi}_k}{\partial t} &= -\frac{1}{2\lambda_k}\,\delta_{\psi_k} \mathcal{H}, \\ \frac{d\lambda_k}{dt} &= 0 \end{aligned}$$

where the bar denotes complex conjugation.

To assess the stability of a given stationary state we employ an energy-Casimir functional

$$\mathcal{H}_C(\psi, \lambda) := \sum_k C(\lambda_k) + \mathcal{H}(\psi, \lambda)$$

with the real-valued function C defined appropriately. Clearly, $\mathcal{H}_C$ is a conserved quantity for the Schrödinger–Poisson system.

The class of functions which generate the Casimir functionals will now be specified: We say that a function $f\colon \mathbb{R} \to \mathbb{R}$ *is of Casimir class* $\mathscr{C}$ iff it has the following properties:

(i) f is continuous with $f(s) > 0, s \leqslant s_0$ and $f(s) = 0, s \geqslant s_0$ for some $s_0 \in \,]0, \infty]$,

(ii) f is strictly decreasing on $]-\infty, s_0]$ with $\lim_{s \to -\infty} f(s) = \infty$,

(iii) there exist constants $\epsilon > 0$ and $C > 0$ such that

$$f(s) \leqslant C(1+s)^{-7/2-\epsilon}, \qquad s \geqslant 0$$

For $f \in \mathscr{C}$,

$$F(s) := \int_s^\infty f(\sigma)\, d\sigma, \qquad s \in \mathbb{R} \tag{2.1}$$

defines a decreasing, continuously differentiable, and non-negative function which is strictly convex on its support, and

$$F(s) \leqslant C(1+s)^{-5/2-\epsilon}, \qquad s \geqslant 0$$

In passing we note that by adjusting various exponents our results easily extend to general space dimensions.

Remark 1. (a) A typical example for $f \in \mathscr{C}$ is the Boltzmann distribution $f(s) = e^{-\beta s}$ with $\beta > 0$, where the cut-off level $s_0 = \infty$. Another example, which also decays exponentially for $s \to \infty$, is given by the Fermi–Dirac statistics:

$$f(s) := C \int_{\mathbb{R}^3} \frac{dv}{\epsilon + e^{|v|^2/2+s}}, \qquad s \in \mathbb{R}$$

where $C > 0$ and $\epsilon > 0$ are positive parameters.

A function f with $f(s) = 0$ for $s > s_0$ with $s_0 \in \mathbb{R}$ will yield a stationary state consisting of a finite number of quantum oscillators.

(b) We could generalize the assumption (iii) to requiring that both $f(-\Delta + V)$ and $F(-\Delta + V)$ are of trace class for (smooth) potentials $V \geqslant 0$, cf. Lemma 1 (b) below. However, we prefer to keep our assumptions on f explicit.

Lemma 1. Let $f \in \mathscr{C}$.

(a) For every $\beta > 1$ there exists $C = C(\beta) \in \mathbb{R}$ such that

$$F(s) \geqslant -\beta s + C, \qquad s \leqslant 0$$

(b) Let $V \in H_0^1(\Omega)$ be non-negative on Ω. Then both $f(-\Delta+V)$ and $F(-\Delta+V)$ are trace class.

Proof. Part (a) is straight forward from assumption (ii) and the definition of F. As to (b), let (μ_k) denote the sequence of eigenvalues of $-\Delta+V$. Then, since V is non-negative and F decreasing,

$$\sum_k F(\mu_k) \leqslant \sum_k F(\mu_k^0)$$

where μ_k^0 denote the eigenvalues of $-\Delta$. For the latter we have the well-known estimate that the number of such eigenvalues less than some $\mu \in \mathbb{R}$ grows like $\mu^{3/2}$ for $\mu \to \infty$, which implies that the right hand sum is finite, and $F(-\Delta+V)$ is trace class. Since f decays faster than F the same holds true for $f(-\Delta+V)$. ▮

At several points the following technical observation will be useful:

Lemma 2. For $\psi \in H_0^1(\Omega) \cap H^2(\Omega)$ with $\|\psi\|_2 = 1$ and $V \in H_0^1(\Omega)$, $V \geqslant 0$, we have

$$F(\langle \psi, (-\Delta+V)\,\psi \rangle) \leqslant \langle \psi, F(-\Delta+V)\,\psi \rangle$$

with equality if ψ is an eigenstate of $-\Delta+V$.

Proof. Denoting the spectral measure associated with $-\Delta+V$ and ψ by $\sigma(d\mu)$ the claim translates into the inequality

$$F\left(\int \mu\sigma(d\mu)\right) \leqslant \int F(\mu)\,\sigma(d\mu)$$

which holds due to the convexity of F and Jensen's inequality. ▮

To conclude this section we make precise the class of stationary states of the Schrödinger–Poisson system considered in this paper: We require that the quadruple $(\psi_0, \lambda_0, \mu_0, V_0)$ with $(\psi_0, \lambda_0) \in \mathscr{S}$, $\mu_0 = (\mu_{0,k}) \in \mathbb{R}^{\mathbb{N}}$, and $V_0 \in H^2(\Omega) \cap H_0^1(\Omega)$ satisfies the stationary Schrödinger–Poisson system

$$(-\Delta+V_0)\,\psi_{0,k} = \mu_{0,k}\psi_{0,k}, \qquad k \in \mathbb{N} \tag{2.2}$$

and

$$\Delta V_0 = -n_0 = -\sum_k \lambda_{0,k}\,|\psi_{0,k}|^2 \tag{2.3}$$

where the energy levels $\mu_{0,k}$ and occupation probabilities $\lambda_{0,k}$ are related through an equation of state of the form

$$\lambda_{0,k} = f(\mu_{0,k}), \qquad k \in \mathbb{N} \tag{2.4}$$

with some $f \in \mathscr{C}$. Note that the corresponding density operator $R_0 = f(-\triangle + V_0)$ satisfies the steady-state Heisenberg equation

$$[H_{V_0}, R_0] = 0$$

We briefly comment on how general the class of these stationary states is:

Remark 2. For a given Hamiltonian $H_V = -\triangle + V$ with an orthonormal basis of eigenfunctions ψ_k and eigenvalues μ_k—each listed according to its multiplicity—the integral kernel of every solution of the operator equation $[H_V, R] = 0$ has the form

$$\sum_{k,\, l;\, \mu_k = \mu_l} \lambda_{kl} \psi_k(x)\, \psi_l(y)$$

cf. ref. 9. If the eigenvalues are all simple—as in the one-dimensional situation—the kernel reduces to $\sum_k \lambda_k \psi_k(x)\, \psi_k(y)$, and in this case $\lambda_k = f(\mu_k)$, $k \in \mathbb{N}$, for some function f. For the stationary states of the Schrödinger–Poisson system which we construct the kernel of the density matrix is of the latter form. Our restrictions on f are such that the resulting stationary states are stable, and one will certainly expect that (possibly unstable) stationary states exist for more general functions f.

Remark 3. If $(\psi_0, \lambda_0, \mu_0, V_0)$ satisfies the equations (2.2), (2.3), (2.4) with $f \in \mathscr{C}$ then the estimate

$$\sum_k \lambda_{0,k} \, \|\psi_{0,k}\|_{H^2}^2 < \infty$$

follows and thus in particular $(\psi, \lambda) \in \mathscr{S}$. To see this we use (2.2) and estimate

$$\sum_k \lambda_{0,k} \, \|\nabla \psi_{0,k}\|_2^2 + \int |\nabla V_0|^2 = \sum_k \mu_{0,k} f(\mu_{0,k}) \leqslant C \sum_k \, (1 + \mu_{0,k})^{-(5/2+\epsilon)} < \infty$$

by assumption (iii) on f and the asymptotic behavior of $\mu_{0,k}$. Thus, by the Sobolev inequality,

$$\|n_0\|_3 \leqslant \sum_k \lambda_{0,k} \, \|\psi_{0,k}\|_6^2 < \infty$$

and $V_0 \in W^{2,3}(\Omega) \subset L^\infty(\Omega)$ follows. Again from (2.2) we conclude that

$$\sum_k \lambda_{0,k} \|\triangle \psi_{0,k}\|_2^2 \leqslant C\left(\sum_k \lambda_{0,k}\mu_{0,k}^2 + \sum_k \lambda_{0,k}\right)$$
$$\leqslant C\left(1 + \sum_k (1+\mu_{0,k})^{-(3/2+\epsilon)}\right) < \infty$$

Remark 4. In the Heisenberg picture the stationary problem (2.2), (2.3) reads

$$\triangle V_0 = -f(-\triangle + V_0)(x, x), \qquad x \in \Omega$$
$$V_0 = 0 \qquad \text{on } \partial\Omega$$

Here and in the sequel we denote by $L(x, y)$ the integral kernel of the trace class operator L.

Given $f \in \mathscr{C}$ we still need to specify the corresponding Casimir functional: With F given by (2.1), its Legendre or Fenchel transform is defined by

$$F^*(s) := \sup_{\lambda \in \mathbb{R}} (\lambda s - F(\lambda)), \qquad s \in \mathbb{R} \tag{2.5}$$

and the energy-Casimir functional corresponding to f is

$$\mathscr{H}_C(\psi, \lambda) := \sum_k F^*(-\lambda_k) + \mathscr{H}(\psi, \lambda), \qquad (\psi, \lambda) \in \mathscr{S} \tag{2.6}$$

Note that since $F' = -f$ has an inverse on $]-\infty, s_0[$,

$$F^*(s) = \int_{-s}^{0} f^{-1}(\sigma)\, d\sigma \tag{2.7}$$

for $-\infty = -f(-\infty) < s \leqslant 0$, and all $-\lambda_k$ lie in this interval.

Obviously, only the values of $f \in \mathscr{C}$ on the interval $]0, \infty[$ are significant for the following theory. However, for technical reasons we consider the functions f defining the equations of state as defined on all of $\mathbb{R}$.

Remark 5. The energy-Casimir functional (2.6) can easily be expressed in the Heisenberg picture. With

$$\widetilde{\mathcal{H}}_C(R) := \operatorname{Tr} F^*(-R) + \operatorname{Tr}(-\triangle R) + \frac{1}{2}\int |\nabla V_R|^2 \, dx$$

where $V_R := V_{\psi,\lambda}$, and R and (ψ, λ) are related by (1.8) we obtain

$$\mathcal{H}_C(\psi, \lambda) = \widetilde{\mathcal{H}}_C(R)$$

Here we have $R \in \widetilde{\mathcal{S}}$, where

$$\widetilde{\mathcal{S}} := \{R : L^2(\Omega) \to L^2(\Omega) | R \geqslant 0, \operatorname{Tr} R + \operatorname{Tr}(-\triangle R) < \infty\}$$

3. STABILITY

In the present section we establish the following result on nonlinear stability in terms of the electrostatic field:

Theorem 1. Let $(\psi_0, \lambda_0, \mu_0, V_0)$ be a stationary state of the Schrödinger–Poisson system with

$$\lambda_{0,k} = f(\mu_{0,k}), \qquad k \in \mathbb{N}$$

for some $f \in \mathscr{C}$, and $(\psi_0, \lambda_0) \in \mathcal{S}$. Then this state is nonlinearly stable in the following sense: If $t \mapsto (\psi(t), \lambda)$ is a solution of the Schrödinger–Poisson system with initial datum $(\psi(0), \lambda) \in \mathcal{S}$ then

$$\tfrac{1}{2} \|\nabla V_{\psi(t),\lambda} - \nabla V_0\|_2^2 \leqslant \mathcal{H}_C(\psi(0), \lambda) - \mathcal{H}_C(\psi_0, \lambda_0), \qquad t \geqslant 0$$

We recall that $\mathcal{H}_C$ is defined by (2.6) for the given function f and note that, clearly, the right hand side in the estimate above becomes arbitrarily small if $(\psi(0), \lambda)$ is close to (ψ_0, λ_0) in the appropriate topology. The main step in the proof of Theorem 1 is to show the following estimate:

Lemma 3. Let $V \in H_0^1(\Omega)$, $V \geqslant 0$. Then

$$\sum_k \left[F^*(-\lambda_k) + \lambda_k \int [|\nabla \psi_k|^2 + V |\psi_k|^2] \right] \geqslant -\operatorname{Tr}[F(-\triangle + V)], \quad (\psi, \lambda) \in \mathcal{S}$$

with equality for $(\psi, \lambda) = (\psi_V, \lambda_V)$, where $\psi_V = (\psi_{V,k}) \in H_0^1(\Omega)^{\mathbb{N}}$ is an orthonormal sequence of eigenfunctions of $-\triangle + V$ with eigenvalues $\mu_V = (\mu_{V,k})$, and $\lambda_V = (\lambda_{V,k}) = (f(\mu_{V,k}))$.

Proof. By (2.5),

$$F^*(-\lambda)+\lambda\mu \geqslant -F(\mu), \qquad \lambda, \mu \in \mathbb{R} \tag{3.1}$$

We substitute λ_k for λ and

$$\mu_k := \int [|\nabla\psi_k|^2 + V\,|\psi_k|^2] = \langle \psi_k, (-\Delta+V)\,\psi_k\rangle$$

for μ and sum over k to find

$$\begin{aligned}\sum_k \Big[F^*(-\lambda_k)+\lambda_k \int [|\nabla\psi_k|^2+V\,|\psi_k|^2]\Big] &\geqslant -\sum_k F(\langle \psi_k, (-\Delta+V)\,\psi_k\rangle)\\ &\geqslant -\sum_k \langle \psi_k, F(-\Delta+V)\,\psi_k\rangle)\\ &= -\mathrm{Tr}[F(-\Delta+V)]\end{aligned}$$

by Lemma 2 and the definition of trace.

Now suppose that $(\psi, \lambda) = (\psi_V, \lambda_V)$. Since by definition each $\psi_{V,k}$ is an eigenfunction of $-\Delta+V$ the μ_k defined above are the corresponding eigenvalues $\mu_{V,k}$, and

$$\mathrm{Tr}[F(-\Delta+V)] = \sum_k F(\mu_{V,k})$$

On the other hand we have $\lambda_{V,k} = f(\mu_{V,k}) = -F'(\mu_{V,k})$ which by conjugacy is equivalent to $\mu_{V,k} = F^{*\prime}(-\lambda_{V,k})$, $k \in \mathbb{N}$. This implies that

$$\sum_k F(\mu_{V,k}) = -\sum_k [F^*(-\lambda_{V,k}) + \lambda_{V,k}\,\mu_{V,k}]$$

and the proof is complete. ∎

Remark 6. In Lemma 3 equality holds if *and only if* $(\psi, \lambda) = (\psi_V, \lambda_V)$. This follows from the strict convexity of F, but we make no use of this observation in the rest of the paper.

Proof of Theorem 1. Let $V = V_{\psi,\lambda}$ be the potential induced by $(\psi, \lambda) \in \mathcal{S}$. Then

$$
\begin{aligned}
&\frac{1}{2}\|\nabla V-\nabla V_0\|_2^2\\
&=\frac{1}{2}\int|\nabla V|^2+\int\triangle V\,V_0+\frac{1}{2}\int|\nabla V_0|^2\\
&=\mathscr{H}_C(\psi,\lambda)-\left[\sum_k\left(F^*(-\lambda_k)+\lambda_k\int|\nabla\psi_k|^2\right)-\frac{1}{2}\int|\nabla V_0|^2-\int\triangle V\,V_0\right]\\
&=\mathscr{H}_C(\psi,\lambda)-\left[\sum_k\left(F^*(-\lambda_k)+\lambda_k\int[|\nabla\psi_k|^2+V_0\,|\psi_k|^2]\right)-\frac{1}{2}\int|\nabla V_0|^2\right]\\
&\leqslant\mathscr{H}_C(\psi,\lambda)-\left[-\mathrm{Tr}[F(-\triangle+V_0)]-\frac{1}{2}\int|\nabla V_0|^2\right]\\
&=\mathscr{H}_C(\psi,\lambda)-\left[\sum_k(F^*(-\lambda_{0,k})+\lambda_{0,k}\int(|\nabla\psi_{0,k}|^2+V_0\,|\psi_{0,k}|^2))-\frac{1}{2}\int|\nabla V_0|^2\right]\\
&=\mathscr{H}_C(\psi,\lambda)-\mathscr{H}_C(\psi_0,\lambda_0)
\end{aligned}
$$

where we have used Lemma 3 twice. Given a solution with $(\psi(0),\lambda)\in\mathscr{S}$ we may substitute $(\psi(t),\lambda)\in\mathscr{S}$ into this estimate, and since $\mathscr{H}_C$ is constant along solutions the assertion follows. ▮

A trivial consequence of Theorem 1 is the following stability estimate for the position density:

$$\tfrac{1}{2}\|n_{\psi(t),\lambda}-n_0\|^2_{H^{-1}(\Omega)}\leqslant\mathscr{H}_C(\psi(0),\lambda)-\mathscr{H}_C(\psi_0,\lambda_0),\qquad t\geqslant 0$$

While our approach does not give a direct estimate for the density matrix, it is possible to refine the estimate (3.1) in Lemma 3 as follows: By Taylor expansion,

$$F^*(-\lambda)+\lambda\mu=F^*(-f(\mu))+f(\mu)\,\mu+\frac{1}{2\,|f'(f^{-1}(\xi(\lambda,\mu)))|}(\lambda-f(\mu))^2 \tag{3.2}$$

where $\xi(\lambda,\mu)$ is between λ and $f(\mu)$, and we assume that $f\in C^1(\mathbb{R})$ with $f'<0$ on $\mathbb{R}$. Adjusting the proof of Theorem 1 accordingly we obtain the following estimate in terms of the wave functions:

Corollary 1. Let the assumptions of Theorem 1 hold and assume in addition that $f\in C^1(\mathbb{R})$ with $f'<0$ on $\mathbb{R}$. Then there exists a constant

$C > 0$ depending on the stationary state such that for any solution of the Schrödinger–Poisson system with, say, $\lambda_k \leqslant \sum_j \lambda_{0,j} + 1$, $k \in \mathbb{N}$,

$$\sum_k |\lambda_k - f(\langle(-\Delta + V_0)\, \psi_k(t), \psi_k(t)\rangle)|^2$$
$$\leqslant C(\mathscr{H}_C(\psi(0), \lambda) - \mathscr{H}_C(\psi_0, \lambda_0)), \qquad t \geqslant 0$$

Note that we are primarily interested in solutions with initial data which are small perturbations of the stationary state, so the size condition on λ_k is not a real restriction.

Proof. Let

$$\mu_k(t) := \langle(-\Delta + V_0)\, \psi_k(t), \psi_k(t)\rangle, \qquad k \in \mathbb{N}, \quad t \geqslant 0$$

Using (3.2) and proceeding as in the proof of Theorem 1 we obtain, with $\xi_k(t)$ between λ_k and $f(\mu_k(t))$,

$$\frac{1}{2} \sum_k \frac{1}{|f'(f^{-1}(\xi_k(t)))|} |\lambda_k - f(\mu_k(t))|^2 + \frac{1}{2} \|\nabla V_{\psi(t),\lambda} - \nabla V_0\|_2^2$$
$$= \mathscr{H}_C(\psi(0), \lambda) - \mathscr{H}_C(\psi_0, \lambda_0)$$

Now $\mu_k(t) \geqslant 0$ so $f(\mu_k(t)) \leqslant f(0)$, $k \in \mathbb{N}$, $t \geqslant 0$. Since by assumption the λ_k are bounded in terms of the stationary state, $0 \leqslant \xi_k(t) \leqslant \gamma$, $k \in \mathbb{N}$, $t \geqslant 0$, with some $\gamma > 0$. If we choose

$$C := 2 \max_{0 \leqslant \xi \leqslant \gamma} |f'(f^{-1}(\xi))| < \infty$$

the assertion follows. ∎

4. DUAL FUNCTIONALS

Our aim for the rest of this paper is to prove the existence of stationary states which satisfy the assumption of our stability result. For each $f \in \mathscr{C}$ a corresponding stationary state will be obtained as the unique maximizer of an appropriately defined functional. In the present section we derive this dual functional from the energy-Casimir functional used in the stability analysis. The relation between these functionals is of interest in itself, but it is not used in the proofs of our results. Throughout this section we fix an element $f \in \mathscr{C}$. We move to the dual functional in two steps. First we apply the saddle point principle and define, for $\Lambda > 0$ fixed,

$$\mathscr{G}(\psi, \lambda, V, \sigma) := \sum_k [F^*(-\lambda_k) + \lambda_k \int [|\nabla \psi_k|^2 + V\, |\psi_k|^2]] - \frac{1}{2} \int |\nabla V|^2 + \sigma \left[\sum_k \lambda_k - \Lambda \right]$$

where $\psi = (\psi_k)$ is again an orthonormal system in $L^2(\Omega)$, $\lambda \in l^1_+ = \{(\sigma_k) \in l^1 \mid \sigma_k \geqslant 0,\ k \in \mathbb{N}\}$, and $V \in H^1_0(\Omega)$ may now vary independently of ψ and λ. The role of the parameter $\sigma \in \mathbb{R}$ (Lagrange multiplier) will become clear shortly; the relation between $\mathscr{H}_C$ and this new functional is as follows:

Remark 7. For any ψ, λ, σ,

$$\sup_V \mathscr{G}(\psi, \lambda, V, \sigma) = \mathscr{H}_C(\psi, \lambda) + \sigma \left[\sum_k \lambda_k - \Lambda \right] \tag{4.1}$$

and the supremum is attained at $V = V_{\psi, \lambda}$. In fact, integration by parts and some computations show that

$$\mathscr{G}(\psi, \lambda, V, \sigma) = \mathscr{H}_C(\psi, \lambda) + \sigma \left[\sum_k \lambda_k - \Lambda \right] - \frac{1}{2} \|\nabla V_{\psi, \lambda} - \nabla V\|_2^2$$

As second step on our way to a dual variational formulation we reduce the functional $\mathscr{G}$ to a functional of V and σ as follows:

$$\Phi(V, \sigma) := \inf_{\psi, \lambda} \mathscr{G}(\psi, \lambda, V, \sigma) \tag{4.2}$$

where the infimum is taken over all $\lambda \in l^1_+$ and all orthonormal sequences ψ in $L^2(\Omega)$. It is this functional which will have a unique maximizer in the next section, which is then a stationary state. First however, we need to bring it into a different form:

Remark 8. The infimum in the definition of Φ is attained at $\psi = (\psi_{V,k})$, an orthonormal sequence of eigenstates of $-\triangle + V$ with corresponding eigenvalues $\mu_{V,k}$, and $\lambda = \lambda_V$ where $\lambda_{V,k} = f(\mu_{V,k} + \sigma)$, $k \in \mathbb{N}$. Moreover,

$$\Phi(V, \sigma) = -\frac{1}{2} \int |\nabla V|^2 - \operatorname{Tr}[F(-\Delta + V + \sigma)] - \sigma \Lambda$$

To see this, recall Lemma 3 and Remark 6 and observe that $f(\cdot+\sigma)\in\mathscr{C}$ for any $\sigma\in\mathbb{R}$, provided $f\in\mathscr{C}$.

Remark 9. In the Heisenberg picture we define

$$\tilde{\mathscr{G}}(R, V, \sigma) := \operatorname{Tr} F^*(-R) + \operatorname{Tr}((-\triangle+V)\, R) - \frac{1}{2}\int |\nabla V|^2\, dx + \sigma(\operatorname{Tr} R - \Lambda)$$

and obtain

$$\tilde{\mathscr{G}}(R, V, \sigma) = \mathscr{G}(\psi, \lambda, V, \sigma)$$

where the density operator's L^2-kernel is given by (1.8).

5. EXISTENCE OF STATIONARY STATES

In the present section we shall for each state relation $f\in\mathscr{C}$ and each total charge $\Lambda>0$ construct a unique maximizer of the functional Φ, which is then a stationary state of the Schrödinger–Poisson system. We consider only non-negative potentials and use the notation

$$H^1_{0,+}(\Omega) := \{V\in H^1_0(\Omega)\mid V\geqslant 0\}$$

Theorem 2. Let $f\in\mathscr{C}$ and $\Lambda>0$ be given. The functional

$$\Phi\colon H^1_{0,+}(\Omega)\times\mathbb{R}\ni(V,\sigma)\mapsto -\frac{1}{2}\int|\nabla V|^2 - \operatorname{Tr}[F(-\Delta+V+\sigma)] - \sigma\Lambda$$

is continuous, strictly concave, bounded from above, and coercive. In particular, there exists a unique maximizer (V_0, σ_0) of Φ. If we define $\psi_0=(\psi_{0,k})$ as the orthonormal sequence of eigenstates of the operator $-\triangle+V_0$ with corresponding eigenvalues $\mu_{0,k}$ and $\lambda_{0,k} := f(\mu_{0,k}+\sigma_0)$, then $(\psi_0, \lambda_0, \mu_0, V_0)$ is a stationary state of the Schrödinger–Poisson system with $\sum_k \lambda_{0,k}=\Lambda$ and $(\psi_0,\lambda_0)\in\mathscr{S}$.

Note that σ_0 plays the role of a (constant) Fermi level here.

Remark 10. In the Heisenberg picture the steady state problem now reads

$$\triangle V_0 = -f(-\triangle+V_0+\sigma_0)(x,x), \qquad x\in\Omega \tag{5.1}$$

$$V_0 = 0 \qquad \text{on } \partial\Omega \tag{5.2}$$

Proof of Theorem 2. *Φ is strictly concave.* The first term of Φ is evidently concave. To show the strict concavity of the second term i.e., the strict convexity of $\mathrm{Tr}[F(-\Delta+V+\sigma)]$, let $(V_j, \sigma_j) \in H^1_{0,+} \times \mathbb{R}$, $j = 1, 2$, $\alpha \in]0, 1[$, and $\phi \in H^2 \cap H^1_0$. By convexity of F and Lemma 2,

$$F(\langle \phi, \alpha(-\Delta+V_1+\sigma_1)\,\phi+(1-\alpha)(-\Delta+V_2+\sigma_2)\,\phi\rangle)$$
$$\leqslant \alpha\langle \phi, F(-\Delta+V_1+\sigma_1)\,\phi\rangle+(1-\alpha)\langle \phi, F(-\Delta+V_2+\sigma_2)\,\phi\rangle$$

Now we substitute ψ_k for ϕ, (ψ_k) an orthonormal sequence of eigenstates of $\alpha(-\Delta+V_1+\sigma_1)+(1-\alpha)(-\Delta+V_2+\sigma_2)$, and sum over k to obtain the convexity estimate for $\mathrm{Tr}[F(-\Delta+V+\sigma]$. If we have equality in this estimate then

$$\langle \psi_k, F(-\Delta+V_1+\sigma_1)\,\psi_k\rangle = \langle \psi_k, F(-\Delta+V_2+\sigma_2)\,\psi_k\rangle, \qquad k \in \mathbb{N}$$

and thus $V_1 = V_2$ and $\sigma_1 = \sigma_2$.

Φ is bounded from above and coercive. Since F is non-negative, the critical case in the coercivity estimate is $\sigma < 0$. Let $\underline{\mu}_V$ denote the ground state energy of $-\Delta+V$ with corresponding ground state $\underline{\psi}_V$. Since F is non-negative and satisfies estimate (a) in Lemma 1 we have for $\sigma \leqslant -\underline{\mu}_V$,

$$\Phi(V, \sigma) \leqslant -\frac{1}{2}\int |\nabla V|^2 - \langle \underline{\psi}_V, F(-\Delta+V+\sigma)\,\underline{\psi}_V\rangle - \sigma\Lambda$$
$$= -\frac{1}{2}\int |\nabla V|^2 - F(-\underline{\mu}_V+\sigma) - \sigma\Lambda$$
$$\leqslant -\frac{1}{2}\int |\nabla V|^2 + (\beta-\Lambda)\,\sigma + \beta\underline{\mu}_V - C$$

where we choose $\beta > \Lambda$. Also

$$\underline{\mu}_V = \inf_{\phi \in H^1_0,\, \|\phi\|_2 = 1} \int [-|\nabla\phi|^2 + V\,|\phi|^2] \leqslant \frac{1}{\mathrm{vol}\,\Omega}\int V \leqslant C_1\,\|V\|_{H^1_0}$$

choosing $\phi := 1/\sqrt{\mathrm{vol}\,\Omega}$. Together with the estimate above and Poincaré's inequality this implies that for $\sigma \leqslant -C_1\,\|V\|_{H^1_0}$ we have

$$\Phi(V, \sigma) \leqslant -C_2\,\|V\|^2_{H^1_0} + C_3\,\|V\|_{H^1_0} + (\beta-\Lambda)\,\sigma + C_4 \tag{5.3}$$

where the constants C_1, C_2, C_3, C_4 are positive and $\beta > \Lambda$, cf. Lemma 1(a). On the other hand, by the non-negativity of F and Poincaré's inequality,

$$\Phi(V, \sigma) \leqslant -C_2 \|V\|^2_{H^1_0} - \sigma\Lambda \tag{5.4}$$

and (5.3) and (5.4) together imply that Φ is bounded from above and coercive.

Existence of a unique maximizer. The existence of a unique maximizer of Φ is standard, cf. for example, ref. 11, Chap. II, Prop. 1.2, provided Φ is upper semi-continuous. This in turn follows from the fact that Φ is concave and bounded from below, at least locally, cf. ref. 11, Chap. I, Lemma 2.1: The only term for which this may not be immediately obvious is the trace term, but

$$\mathrm{Tr}[F(-\Delta + V + \sigma)] \leqslant \sum_k F(\mu_k + \sigma_0) < \infty$$

where μ_k are the eigenvalues of $-\Delta + V$ and $\sigma \geqslant \sigma_0$ for arbitrary $\sigma_0 \in \mathbb{R}$.

$(\psi_0, \lambda_0, \mu_0, V_0)$ is a stationary state. Since $F' = -f$, the stationarity of $\Phi(V_0, \sigma)$ with respect to σ implies

$$0 = \left.\frac{d\Phi(V_0, \sigma)}{d\sigma}\right|_{\sigma_0} = \mathrm{Tr}[f(-\Delta + V_0 + \sigma_0)] - \Lambda$$

$$= \sum_k f(\mu_{0,k} + \sigma_0) - \Lambda = \sum_k \lambda_{0,k} - \Lambda$$

so that $\sum_k \lambda_{0,k} = \Lambda$ as claimed. In order that $(\psi_0, \lambda_0, \mu_0, V_0)$ is a stationary state we need to show that

$$\Delta V_0 + \sum_k \lambda_{0,k} |\psi_{0,k}|^2 = 0 \tag{5.5}$$

To verify this we observe that V_0, being a maximizer of $\Phi(\cdot, \sigma_0)$, satisfies the Euler–Lagrange equation (5.1). In our case

$$f(-\Delta + V_0 + \sigma_0)(x, x) = \sum_k f(\mu_{0,k} + \sigma_0) |\psi_{0,k}|^2 (x) \tag{5.6}$$

and (5.5) follows from (5.1), (5.6), and the fact that by definition, $\lambda_{0,k} = f(\mu_{0,k} + \sigma_0)$. As to the proof for $(\psi_0, \lambda_0) \in \mathcal{S}$ we refer to Remark 3. ∎

In view of the relations between our various functionals derived in the previous section it is of interest to note:

Remark 11. If (V_0, σ_0) is the maximizer obtained in Theorem 2 and $(\psi_0, \lambda_0, \mu_0, V_0)$ is the corresponding stationary state, then

$$\Phi(V_0, \sigma_0) = \mathcal{H}_C(\psi_0, \lambda_0)$$

To see this, note that by (4.2) we have

$$\Phi(V_0, \sigma_0) = \mathcal{G}(\psi_0, \lambda_0, V_0, \sigma_0) \leqslant \mathcal{H}_C(\psi_0, \lambda_0)$$

where equality holds iff V_0 is the maximizer of $\mathcal{G}(\psi_0, \lambda_0, V, \sigma_0)$ on H_0^1; note that here $\mathcal{G}$ is independent of σ since $\sum_k \lambda_{0,k} = 1$. This, on the other hand, is equivalent to the fact that V_0 is the solution of the Poisson equation (5.5).

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