Existence and Nonlinear Stability of Stationary States of HP System

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I Introduction and Preliminaries

The purpose of this report is to rephrase the results and approach of the paper, *Existence and Nonlinear Stability of Stationary States of the Schrodinger-Poisson System* [1], in the Heisenberg picture of Quantum Mechanics.

To begin, let us state the problem. We consider a large ensemble of n-charged quantum particles confined to the spatial domain $\Omega \subset \mathbb{R}^3$ that interact only via the electrostatic field they collectively create. We assume Ω is bounded with sufficiently smooth boundary. An effective model for this system is the Hartree problem:

$$i\frac{\partial R}{\partial t} = [H_V, R] \tag{I.1}$$

$$H_V := -\Delta + V(t,x) \tag{I.2}$$

$$\Delta V = -n \tag{I.3}$$

$$n(t,x) = R(t,x,x) \tag{I.4}$$

Here $R(t)$ denotes the density operator of the system, a time-dependent, hermitian, positive trace class operator acting on the Hilbert space $L^2(\Omega)$. Equation (I.1) is the Von Neumann-Heisenberg equation with Hamiltonian H_V. The potential V is a solution to the Poisson equation (I.3) subject to homogeneous Dirichlet boundary condition:

$$V(t,x) = 0$$

for $t \geqslant 0, x \in \partial\Omega$. 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 $n(t,x)$. We shall refer to this system as the *Heisenberg-Poisson System* (HP).

We thus consider the solution space for the system to be the set

$$\mathcal{P} := \{R : L^2(\Omega) \to L^2(\Omega) | R \geqslant 0, TrR + Tr(-\Delta R) < \infty\}$$

This system has energy functional

$$\mathcal{H}(R) := Tr(-\Delta R) + \frac{1}{2}\int |\nabla V_R|^2$$

where V_R is related to R by the Poisson equation (I.3). It turns out that this energy functional will not be sufficient for our analysis, as the total energy of the system is conserved along solutions but the stationary states are not critical points of the energy. However, there exist additional conserved quantities, named Casimir functionals [2], created so that a given stationary state is a critical point for the respectively chosen energy-plus-Casimir functional. We shall call this functional $\mathcal{H}_C$. Let us now define them.

The Casimir functionals will be generated from a class of functions $\mathcal{C}$. A function $f : \mathbb{R} \to \mathbb{R}$ is of Casimir class $\mathcal{C}$ if and only if it has the following properties:

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

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

3) there exists a constants $\epsilon > 0$ and $C > 0$ such that for $s \geqslant 0$,

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

For a function $f \in \mathcal{C}$, we define

$$F(s) = \int_s^\infty f(\sigma)d\sigma$$

for all $s \in \mathbb{R}$. This defines a decreasing, continuously differentiable, non-negative function that is strictly convex on its support. Furthermore we have the bound:

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

for $s \geqslant 0$. which follows trivially from the third property of f. We may now define the Casimir energy functional. For a function F defined as a above, its Legendre-Fenchel transform is defined by

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

for all $s \in \mathbb{R}$. Thus, the Casimir energy functional corresponding to a function f is defined as:

$$\mathcal{H}_C(R) := TrF^*(-R) + Tr(-\Delta R) + \frac{1}{2} \int |\nabla V_R|^2$$

Before defining the class of stationary states and moving onto the main results of the paper, we discuss and prove some technical lemmas which will be useful.

Lemma 1. Let $f \in \mathcal{C}$. Then:

a) For every $\beta > 1$ there exists $C = C(\beta) \in \mathbb{R}$ such that for $s \leqslant 0$

$$F(s) \geqslant -\beta s + C$$

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 of Lemma 1. Proof of a) This follows from condition 2) that allows $f \in \mathcal{C}$, by observing that F is decreasing and convex.
Proof of b) Let (μ_k) denote the sequence of eigenvalues of $-\Delta + V$, and (μ_k^0) the eigenvalues of $-\Delta$. Since V is positive, then by the min-max principle we have:

$$\begin{aligned}
\mu_k^0 &= \min_{\phi_0,\ldots,\phi_N} \max_{\phi} \{\langle \phi, (-\Delta)\phi \rangle : \phi \in span\{\phi_0, \ldots, \phi_N\}\} \\
&\leq \min_{\phi_0,\ldots,\phi_N} \max_{\phi} \{\langle \phi, (-\Delta + V)\phi \rangle : \phi \in span\{\phi_0, \ldots, \phi_N\}\} = \mu_k
\end{aligned}$$

where $\langle \phi, \phi \rangle = 1$. And hence, since F is decreasing,

$$\begin{aligned}
TrF(-\Delta + V) &= \sum_k F(\mu_k) \\
&\leq \sum_k F(\mu_k^0) = TrF(-\Delta)
\end{aligned}$$

The right hand sum is finite by the well-known quasiclassical bound

$$TrF(-\Delta) \leq \int F(|\xi|^2) dx d\xi$$

and hence $F(-\Delta+V)$ is trace class. Since f decays faster than F we conclude that $f(-\Delta+V)$ is also trace class. $\square$

Lemma 2. For $\psi \in H_0^1(\Omega) \cup H^2(\Omega)$ 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 of Lemma 2. We may denote the spectral measure associated with $-\Delta+V$ and ψ by $\sigma(d\mu)$. Then we may re-write the inequality in the following form:

$$F(\int \mu \sigma(d\mu)) \leqslant \int F(\mu)\sigma(d\mu)$$

Using the fact that F is convex then this is directly Jensen's inequality. $\square$

We are now ready to define the class of stationary states. We define a stationary state the pair (R_0, V_0) where for $x \in \Omega$:

$$\Delta V_0 = -f(-\Delta+V_0)(x,x)$$

(ie. the L^2-integral kernel) for some $f \in \mathcal{C}$, with Dirichlet boundary condition $V_0 = 0$ on $\partial\Omega$. In other words, the density operator is defined as

$$R_0 := f(-\Delta+V_0)$$

Note that it satisfies the steady-state Heisenberg equation

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

We can see that R_0 is positive and trace class by Lemma 1.

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

$$Tr(F^*(-R)) + Tr(HR) \geqslant -Tr[F(H)]$$

for $R \in \mathcal{P}$. We have equality if $R = f(H)$, where recall $H = -\Delta+V$.

Proof of Lemma 3. First we show the inequality. From the definition of the Legendre-Fenchel transform, we have

$$F^*(-\lambda) + \lambda\mu \geqslant -F(\mu) \tag{I.5}$$

Let λ_k, ϕ_k denote the eigenvalues and eigenfunctions of R, respectively. Then,

$$\begin{aligned}
Tr(F^*(-R) + HR) &= \sum_k \langle \phi_k, (F^*(-R) + HR)\phi_k \rangle \\
&= \sum_k \langle \phi_k, (F^*(-\lambda_k) + H\lambda_k)\phi_k \rangle) \\
&\geqslant \sum_k \langle \phi_k, -F(H)\phi_k \rangle \\
&= -TrF(H)
\end{aligned}$$

where to obtain the first inequality we have used (I.5). Hence, we have proved the inequality. To prove the equality case, observe that if $R = f(H)$ then ϕ_k are also eigenvectors of H as it commutes with R. Denote the eigenvalues of H by μ_k. Then,

$$\begin{aligned}
Tr(F^*(-R) + HR) &= \sum_k \langle \phi_k, (F^*(-R) + HR)\phi_k \rangle \\
&= \sum_k \langle \phi_k, (F^*(-f(\mu_k)) + \mu_k\lambda_k)\phi_k \rangle) \\
&= \sum_k \langle \phi_k, -F(\mu_k)\phi_k \rangle \\
&= -TrF(H)
\end{aligned}$$

using the conjugacy of the L-F transform (ie. $F = F^{**}$). □

II Stability

We are now ready to discuss the main stability result of the paper. It should be noted that this is not a direct result on the density operator.

Theorem A. Denote (R_0, V_0) a stationary state of the HP system, so that $R_0 = f(H_0)$ for some $f \in \mathcal{C}$, $R_0 \in \mathcal{P}$. This solution is then nonlinearly stable in the following sense: let $R(t)$ denote a solution of the HP system with initial datum $R(0) \in \mathcal{P}$. Then,

$$\frac{1}{2}\|\nabla V(t) - \nabla V_0\|_2^2 \leqslant \mathcal{H}_C(R(0)) - \mathcal{H}_C(R_0)$$

Observe that the right hand side becomes arbitrarily small if $R(0)$ is sufficiently close to R_0 in the right topology (**). We may rephrase this result in terms of the position density using the dual norm:

$$\frac{1}{2}\|n(t) - n_0\|_{H^{-1}(\Omega)}^2 \leqslant \mathcal{H}_C(R(0)) - \mathcal{H}_C(R_0)$$

Proof of Theorem A. Observe that,

$$\begin{aligned}
\frac{1}{2}\|\nabla V(t) - \nabla V_0\|_2^2 &= \frac{1}{2}\int |\nabla V(t)|^2 + \int \Delta V(t) V_0 + \frac{1}{2}\int |\nabla V_0|^2 \\
&= \mathcal{H}_C(R(t)) - [TrF^*(-R(t)) + Tr(-\Delta R(t)) - \int \Delta V(t) V_0 \\
&\quad - \frac{1}{2}\int |\nabla V_0|^2] \\
&= \mathcal{H}_C(R(t)) - [TrF^*(-R(t)) + Tr(H_0)R(t) - \frac{1}{2}\int |\nabla V_0|^2]
\end{aligned}$$

We now use Lemma 3 twice, the second time as equality (for stationary solutions) and obtain the bound:

$$\begin{aligned}
\frac{1}{2}\|\nabla V(t) - \nabla V_0\|_2^2 &\leqslant \mathcal{H}_C(R(t)) - [-TrF(-\Delta + V_0) - \frac{1}{2}\int |\nabla V_0|^2] \\
&= \mathcal{H}_C(R(t)) - [TrF^*(-R_0) + Tr(H_0)R_0 - \frac{1}{2}\int |\nabla V_0|^2] \\
&= \mathcal{H}_C(R(t)) - \mathcal{H}_C(R_0)
\end{aligned}$$

□

III Existence

We now seek to prove the existence of these stationary states as minimizers of appropriately chosen functionals. We obtain for each $f \in \mathcal{C}$ a stationary state, minimizing a functional directly derived from the corresponding

Casimir-energy functional. We first derive this corresponding energy functional, and then prove the existence of stationary states.

We first make use of the saddle-point principle and for $\sigma \in \mathbb{R}$ lagrange multiplier define the functional

$$\begin{aligned}\mathcal{G}(R,V,\sigma) &:= TrF^*(-R) + Tr[F(-\Delta+V)R] - \frac{1}{2}\int |\nabla V|^2 + \sigma(TrR - \Lambda) \\ &= TrF^*(-R) + Tr[F(-\Delta+V+\sigma)R] - \frac{1}{2}\int |\nabla V|^2 - \sigma\Lambda\end{aligned}$$

where Λ can be interpreted as the total charge. Observe that the function $f(\cdot+\sigma)$ is still Casimir class $\mathcal{C}$. Thus by Lemma 3 we obtain a minimized functional over R with minimizer $R_0 = f(-\Delta+V+\sigma)$, since

$$\mathcal{G}(R,V,\sigma) \geqslant -TrF(-\Delta+V+\sigma) - \frac{1}{2}\int |\nabla V|^2 - \sigma\Lambda$$

We thus define the functional

$$\begin{aligned}\Phi(V,\sigma) &:= \inf_R \mathcal{G}(R,V,\sigma) = \mathcal{G}(R_0,V,\sigma) \\ &= -\frac{1}{2}\int |\nabla V|^2 - Tr[F(-\Delta+V+\sigma)] - \sigma\Lambda\end{aligned}$$

The main existence result is constructing for each state relation $f \in \mathcal{C}$ and total charge $\Lambda > 0$ a unique maximizer of the functional Φ and showing that this is a stationary state of the HP system. In order to prove this result we shall make use of a few standard results in the minimization of convex functions. Our reference will be Ekeland-Temam [3].

Lemma 4 (Lemma 2.1 in Chapter 1 of [3])**.** Consider a function F defined on a Banach space V. If F in a neighbourhood of $u \in V$ is convex and bounded above by a finite constant, then F is continuous at u.

Proof of Lemma 4. By translation, without loss of generality we can assume $u = 0$ and $F(0) = 0$. Let U be a neighbourhood of the origin such that $F(u) \leqslant a < \infty$ for all $u \in U$. Define the set

$$W = U \cap -U$$

where $-U$ is the symmetric reflection of U around the origin. Let $\epsilon \in (0,1)$. If $v \in \epsilon W$, then by the convexity of F, we have two possibilities:

If $\frac{v}{\epsilon} \in U$ then $F(v) \leqslant (1-\epsilon)F(0) + \epsilon F(\frac{v}{\epsilon}) \leqslant \epsilon a$

If $-\frac{v}{\epsilon} \in U$ then $F(v) \geqslant (1+\epsilon)F(0) - \epsilon F(-\frac{v}{\epsilon}) \geqslant -\epsilon a$

Thus we have that $|F(v)| \leqslant \epsilon a$ for all $v \in \epsilon W$, and so continuity of F at $u = 0$ follows. □

Lemma 5 (Proposition 1.2 in Chapter 2 of [3])**.** Assume F is a function, defined on a domain Ω in a reflexive Banach space V convex, lower-semicontinuous and proper. Then, if the domain is bounded or F is coercive, ie

$$\lim F(u) \to \infty \text{ as } \|u\| \to \infty$$

then $\inf_u F(u)$ has a solution, which is unique if F is strictly convex.

Proof of Lemma 5. Existence: Let $\{u_\alpha\}$ be a minimizing sequence for F, ie

$$F(u_\alpha) \to \inf_u F(u) = a \text{ as } \alpha \to \infty$$

We want to show that $\alpha \neq -\infty$. Note that $\{u_\alpha\}$ is bounded in V. This follows directly from the fact that the domain Ω is bounded, or from the fact that the sequence $F(u_\alpha)$ is bounded above from coercivity. Thus, we have a weakly convergent subsequence u_{α_i} (recall that we assumed V reflexive) in V to $u \in \Omega$. It follows that since F is convex it is also lower-semicontinuous on V with the weak topology (we shall use this fact without proof). Hence,

$$F(u) \leqslant \liminf_{\alpha_i \to \infty} F(u_{\alpha_i}) = a$$

So, u is a minimizer.

Uniqueness If we have two different minimizers u_1 and u_2, then since the set of solutions to the minimization problem is convex (and possibly empty - again, a fact we shall use without proof, although the proof is not difficult) then $\frac{1}{2}(u_1 + u_2)$ is also a minimizer. Hence, if F is strictly convex, by this strict convexity we have:

$$F(\frac{1}{2}(u_1 + u_2)) < \frac{1}{2}[F(u_1) + F(u_2)] = a$$

so we arrive at a contradiction. Thus, there cannot be more than one minimizer if F is strictly convex. □

We are now ready to state the main existence theorem. Consider only non-negative potentials, using the notation $H^1_{0,+} := \{V \in H^1_0(\Omega) : V \geqslant 0\}$, where recall H^1_0 is the space of H^1 functions with Dirichlet boundary conditions on $\delta\Omega$ (this interpretation is valid in light of considering domains Ω with sufficiently smooth boundary).

Theorem B. For $f \in \mathcal{C}$ and $\Lambda > 0$, the functional

$$\Phi(V,\sigma) : H^1_{0,+}(\Omega) \times \mathbb{R} \to \mathbb{R}$$

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

is continuous, strictly concave, bounded from above and coercive. In particular there exists a unique maximizer of (V_0, σ_0) of Φ. The corresponding density operator $R_0 := f(-\Delta + V_0 + \sigma_0)$ is a stationary state of the HP system with $TrR_0 = \Lambda$ and $R_0 \in \mathcal{P}$.

Proof of Theorem B. Φ is strictly concave: First observe that the first term is concave as the term $\int|\nabla V|^2$ is convex. Indeed, for all $\alpha \in [0,1]$:

$$\begin{aligned}\int |\nabla(\alpha V_1 + (1-\alpha)V_2)|^2 &= \int |\alpha \nabla V_1|^2 + 2\alpha\nabla V_1 \cdot (1-\alpha)\nabla V_2 + |(1-\alpha)\nabla V_2|^2 \\ &\leqslant \int |\alpha\nabla V_1|^2 + |(1-\alpha)\nabla V_2|^2 \\ &< \int \alpha|\nabla V_1|^2 + (1-\alpha)|\nabla V_2|^2\end{aligned}$$

since $\alpha, (1-\alpha)$ are both less than or equal to one. The third term $-\sigma\Lambda$ is obviously concave. Thus, it remains to show the strict concavity of the second term, ie. the strict convexity of $Tr[F(-\Delta + V + \sigma)]$. We make use of the fact that F is convex. Let $(V_1, \sigma_1), (V_2, \sigma_2) \in H^1_{0,+} \times \mathbb{R}$ and $\alpha \in (0,1)$. To simplify notation, denote $-\Delta + V_i + \sigma_i$ by H_i. Denote the sequence of eigenstates of $\alpha H_1 + (1-\alpha)H_2$ by (ψ_k). Then, using the orthonormality of eigenfunctions to re-insert them inside F,

$$\begin{aligned}
Tr[F(\alpha H_1 + (1-\alpha)H_2)] &= \sum_k \langle \psi_k, F(\alpha H_1 + (1-\alpha)H_2)\psi_k\rangle \\
&= \sum_k F(\langle \psi_k, (\alpha H_1 + (1-\alpha)H_2)\psi_k\rangle) \\
&\leqslant \sum_k \alpha F(\langle \psi_k, H_1\psi_k\rangle) + (1-\alpha)F(\langle \psi_k, H_2\psi_k\rangle) \\
&\leqslant \alpha Tr[F(H_1)] + (1-\alpha)Tr[F(H_2)]
\end{aligned}$$

If we have equality in this estimate, then by the strict convexity of F on its support,

$$\langle \psi_k, F(H_1)\psi_k\rangle = \langle \psi_k, F(H_2)\psi_k\rangle$$

so thus $V_1 = V_2$ and $\sigma_1 = \sigma_2$, so we obtain strict convexity of the term $Tr[F(-\Delta + V + \sigma)]$.

Φ *is coercive and bounded from above*: We seek the show that Φ is coercive:

$$\Phi \to -\infty \text{ as } \|V\|^2_{H^1_0} \text{ and } |\sigma| \to \infty$$

Observe that F is non-negative for all values in its domain. Hence,

$$\Phi \leqslant -C_2\|V\|^2_{H^1_0} - \sigma\Lambda \tag{III.1}$$

where we have used Poincare's inequality. The conditions follow except in the case that $\sigma < 0$ as $|\sigma| \to \infty$. In this case we require an additional inequality. Consider the ground state energy of $-\Delta + V$ denoted by μ_V. Then μ_V is the solution of the variational problem:

$$\mu_V = \inf_{\phi \in H^1_0, \|\phi\|_2 = 1} \int (-|\nabla\phi|^2 + V|\phi|^2)$$

We thus obtain a relatively simple bound for μ_V by choosing $\phi = \frac{1}{\sqrt{Vol\Omega}}$, so

$$\mu_V \leqslant \frac{1}{Vol\Omega}\int V \leqslant C_1\|V\|_{H^1_0}$$

Now, using the fact that F is non-negative,

$$\begin{aligned}
\Phi &\leqslant -\frac{1}{2}\int |\nabla V|^2 - F(-\mu_V + \sigma) - \sigma\Lambda \\
&\leqslant -\frac{1}{2}\int |\nabla V|^2 + (\beta - \Lambda)\sigma + \beta\mu_V - C(\beta)
\end{aligned}$$

where for the second inequality we have used part a) of Lemma 1 for $\sigma \leqslant -\mu_V$, choosing $\beta > \lambda$. Then, combining this with the bound on μ_V and apply Poincare's Lemma again, we have our second inequality on Φ:

$$\Phi \leqslant -C_2\|V\|_{H_0^1}^2 + C_3\|V\|_{H_0^1} + (\beta - \Lambda)\sigma + C_4 \tag{III.2}$$

for $\sigma \leqslant -C_1\|V\|_{H_0^1}$. Observe that all the constants are positive, including $\beta - \Lambda$. Hence, it now follows that Φ is coercive. We can conclude Φ is bounded from above in both cases. In the case where $\sigma \geqslant 0$, we have the bound $\Phi \leqslant 0$ via equation (III.1). Similarily, in the negative case we can use equation (III.2) to obtain the bound

$$\Phi \leqslant \frac{C_3}{2C_2} + C_4$$

Hence Φ is bounded from above.

Existence of a unique Maximizer: We seek to use Lemma 5 directly. We may conclude the existence of a unique maximizer of $\Phi(V, \sigma)$ by showing it is additionally upper semi-continuous. We actually obtain local continuity via Lemma 4. In order to do so we seek to show that Φ is concave and bounded below by a finite constant. We have concavity from previous arguments, and local boundedness for the first and last terms is obvious. For the trace term, recall that $F(-\Delta + V + \sigma)$ is trace-class as remarked previously, and hence the trace term is bounded below. Thus we have the existence of a unique (by the strict concavity of Φ) maximizer of $\Phi(V, \sigma)$, which we denote (V_0, σ_0).

Corresponding density operator is a Stationary State: The corresponding density operator is defined by

$$R_0 := f(-\Delta + V_0 + \sigma_0)$$

First observe the stationary problem is now:

$$\Delta V_0 = -f(-\Delta + V_0 + \sigma_0)(x, x)$$

with Dirichlet boundary conditions. Since V_0 is a maximizer of $\Phi(\cdot, \sigma_0)$ the above equation amounts to the E-L equation for Φ in the variable V:

$$\begin{aligned} 0 &= \frac{d\Phi(V, \sigma_0)}{dV}\Big|_{V=V_0} \\ &= Re \int (\Delta V_0(x) + f(-\Delta + V_0 + \sigma_0)(x, x)) \end{aligned}$$

Thus (R_0, V_0) is a stationary state. We also have $-\Delta R_0$ trace-class hence $Tr(-\Delta R_0)$ is finite. It thus follows that $R_0 \in \mathcal{P}$. On the other hand, the E-L equations in σ yield:

$$\begin{aligned} 0 &= \frac{d\Phi(V_0,\sigma)}{d\sigma}\Big|_{\sigma=\sigma_0} \\ &= Tr[f(-\Delta + V_0 + \sigma_0)] - \Lambda \\ &= Tr R_0 - \Lambda \end{aligned}$$

where we used the fact that $F' = -f$. Hence, $Tr R_0 = \Lambda$. $\square$

References

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