On Asymmetric Quasiperiodic Solutions of Hartree-Fock Systems

by

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ABSTRACT

The time-dependent Hartree-Fock system is considered in the presence of external magnetic and electric fields, and with a self-consistent potential including anisotropies. A suitable ansatz reduces a quasiperiodic time-dependent problem to an eigenvalue problem, which is then solved by minimization of an energy functional.

1. Introduction. We are concerned with solutions of the Hartree-Fock system (see, e.g., [3]) in two space dimensions, in the presence of a constant magnetic field (vector potential) $\vec{A}(x) = \omega(-x_2, x_1)$ with field strength $\omega > 0$ and an external electric potential $U_0(x_1, x_2) = \frac{1}{2}\rho_0|x|^2$ (constraints on ρ_0 are given below).

This problem models a beam of spinless quantum particles satisfying the Pauli principle; the beam is confined by the magnetic field and the external electric field. It will be transparent from our analysis that the choice of the isotropic electric external potential is only an example of a larger admissible class of isotropic external potentials; the key point is that the electric potential cannot overcome the magnetic confinement of the beam.

By the same token, the method will be seen to generalize to three dimensions. All that is needed is a third (confining) component to the electric field, which will prevent the particle system from escaping in the third coordinate direction. We will do the rigorous analysis for the two-dimensional situation and then cover the three-dimensional case by comments.

Variational methods are classical for proving the existence of stationary solutions of the Hartree-Fock system (without imposing *a priori* anisotropy: see [1], [7], [8]). Our research was inspired by similar results obtained for the classical Vlasov-Poisson system (see [2]).

The type of Hamiltonian which we encounter in our study arises, e.g., in the study of quantum dots (see, e.g., [10] for a recent survey).

We denote $x = (x_1, x_2)$, $|x|^2 = x_1^2 + x_2^2$. The full Hartree-Fock system is the nonlinearly coupled system for countably many wave functions φ_l, $l = 1, 2, \ldots$, dependent on x and t,

$$\begin{aligned} i\hbar\partial_t\varphi_l = {} & \frac{1}{2m}(-i\hbar\nabla_x - \frac{q}{c}\vec{A}(x))^2\varphi_l + qU[n]\varphi_l \\ & + q\sum_{j=1}^{\infty}\lambda_j V_{lj}\varphi_j + q\frac{\rho_0}{2}|x|^2\varphi_l. \end{aligned} \tag{1.1}$$

Here, q is the charge of a spinless quantum particle, m is its mass, $\hbar$ is the Planck constant and c is the velocity of light. The $\lambda_j s$ in (1.1) are probabilities that the system finds itself in the state φ_l at time t, where φ_l is the eigenfunction of the density matrix associated with the eigenvalue λ_l. The system (1.1) is one of three common and equivalent descriptions of the time evolution of ensembles of spinless quantum particles obeying the Pauli principle; the other two are the Heisenberg and Wigner descriptions (see [4]). In (1.1), $n(x,t) = \sum \lambda_j |\varphi_j(x,t)|^2$, and the self-consistent potential $U[n]$ is coupled with n via the Poisson equation

$$-\Delta U(\cdot,t) = n(\cdot,t). \tag{1.2}$$

The relevant solutions of (1.2) in two dimensions are

$$U(x,t) = -\frac{1}{2\pi}\int \ln|x-y|\, n(y,t)\; dy + U_1(x,t),$$

where $\Delta U_1(\cdot,t) = 0$. (if n decays fast enough for the integral to e xist). The Pauli correction V_{lj} is given by

$$V_{lj}(x,t) = \frac{1}{2\pi}\int \ln|x-y|\; \varphi_l(y,t)\bar{\varphi}_j(y,t)\, dy. \tag{1.3}$$

Equation (1.1) can be written as

$$\begin{aligned} i\hbar\partial_t\varphi_l = {} & \frac{-\hbar^2}{2m}\Delta_x\varphi_l + \frac{i\hbar q\omega}{mc}(-x_2\partial_{x_1} + x_1\partial_{x_2})\varphi_l + qU[n]\varphi_l \\ & + q\sum_{j=1}^{\infty}\lambda_j V_{lj}\varphi_j + q\frac{\rho_0 + \omega^2\frac{q}{mc^2}}{2}|x|^2\varphi_l. \end{aligned} \tag{1.4}$$

To simplify our analysis, we now set all the physical constants $\hbar, m, c$ and q equal to one (the general case follows in complete analogy). Eqn. (1.4) simplifies to

$$\begin{aligned} i\partial_t\varphi_l = {} & \frac{-1}{2}\Delta_x\varphi_l + i\omega(-x_2\partial_{x_1} + x_1\partial_{x_2})\varphi_l + U[n]\varphi_l \\ & + \sum_{j=1}^{\infty}\lambda_j V_{lj}\varphi_j + \frac{\rho_0 + \omega^2}{2}|x|^2\varphi_l. \end{aligned} \tag{1.5}$$

Moreover, we consider (1.4) under the assumption that $\omega^2 + \rho_0 > 0$. We set $\delta = \rho_0 + \omega^2$ and equation (1.5) r eads

$$\begin{aligned} i\partial_t\varphi_l = {} & \frac{-1}{2}\Delta_x\varphi_l + i\omega(-x_2\partial_{x_1} + x_1\partial_{x_2})\varphi_l + U[n]\varphi_l \\ & - \sum_{j=1}^{\infty}\lambda_j V_{lj}\varphi_j + \frac{\delta}{2}\left(x_1^2 + x_2^2\right)\varphi_l, \end{aligned} \tag{1.6}$$

with $\Delta U = -n$.

We next reduce the problem further by looking only for a special class of periodic solutions. To this end, let R_ω denote the rotation matrix in counter-clockwise direction by the angle $\pi/4$, and with angular velocity ω :

$$R_\omega = \omega \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Then

$$\exp(tR_\omega)x = \begin{pmatrix} \cos(\omega t)x_1 - \sin(\omega t)x_2 \\ \sin(\omega t)x_1 + \cos(\omega t)x_2 \end{pmatrix}$$

and for any sufficiently smooth function f, $(x,t) \to f(\exp(tR_\omega)x)$ solves

$$\partial_t \varphi = \omega(-x_2\partial_{x_1} + x_1\partial_{x_2})\varphi \tag{1.7}$$

(i.e., the differential operator on the right of (1.7) generates a rotation group). This motivates the ansatz

$$\varphi_l(x,t) = e^{-iE_l t}\psi_l(e^{tR_\omega}x) \tag{1.8}$$

to solve (1.6), and by inspection one proves

Theorem 1. *The family of functions given by (1.8) solves (1 .6) if and only if $\Psi := (\psi_l)_{l=1,2,...}$ satisfy the coupled eigenfunctio n equations*

$$E_l\psi_l = -\frac{1}{2}\Delta\psi_l + U[n]\psi_l + \sum_j \lambda_j V_{lj}\psi_j + \frac{\delta}{2}\left(x_1^2 + x_2^2\right)\psi_l \tag{1.9}$$

with $-\Delta U = n = \sum \lambda_l |\psi_l|^2$, *i.e.,* $U(x) = -\frac{1}{2\pi}\int \ln|x-y|\, n(y)\, dy + U_1(x)$ *with* $\Delta U_1 = 0$, *and*

$$V_{lj}(x) = \int \ln|x-y|\, \psi_l(y)\bar{\psi}_j(y)\, dy. \tag{1.10}$$

In the remainder of this paper, we solve (1.9-10) by minimizing an energy functional. Notice that U is only determined up to a harmonic contribution component U_1 of the self-consistent potential (with a slight abuse of notation, we use the notations U and U_1 even even after making the ansatz (1.8);

U and U_1 do now not depend on t anymore). The trivial choice $U_1 = 0$ leads to isotropic eigenstates. We will treat the more general situation where $U_1 = \frac{\tilde{\theta}}{2}(x_1^2 - x_2^2)$, which leads to anisotropy if $\tilde{\theta} > 0$. Note that $\Delta U_1 = 0$, i.e., U_1 is an admissible correction to the self-consistent potential. To guarantee confinement, we have to restrict ourselves to the weak anisotropy situation where $0 \leq \tilde{\theta} < \delta$ (the case $-\delta < \theta \leq 0$ follows then by exchanging x_1 with x_2). Setting $\tilde{\theta} = \theta\delta$, Eqn. (1.9) becomes

$$E_l\psi_l = -\frac{1}{2}\Delta\psi_l + U[n]\psi_l + \sum_j \lambda_j V_{lj}\psi_j + \frac{\delta}{2}\left((1+\theta)x_1^2 + (1-\theta)x_2^2\right)\psi_l \quad (1.11)$$

with $U[n] = -\frac{1}{2\pi}\int \ln|x-y| n(y)\, dy$.

2. Solving the eigenvalue problem. We first recall the representation of the density matrix ρ in terms of its eigenfunctions:

$$\rho(x,y,t) = \sum \lambda_l \bar{\varphi}_l(x,t)\varphi_l(y,t). \quad (2.1)$$

Next, we define an energy functional for the system (1.11) by

$$\begin{aligned}\mathcal{E}(\Psi) :=& \frac{1}{4}\sum_l \lambda_l \int |\nabla\psi_l(x)|^2 dx \\ &- \frac{1}{4\pi}\int\int \ln|x-y| \left(n(x)n(y) - |\rho(x,y)|^2\right) dxdy \\ &+ \frac{\delta}{2}\int \left((1+\theta)x_1^2 + (1-\theta)x_2^2\right) n(x)\, dx.\end{aligned} \quad (2.2)$$

Let a function space $\mathbb{Y}$ be defined by

$$\mathbb{Y} = \{\Psi; \quad \psi_l \in L^2 \cap H^1, \quad \sum \lambda_l \|\psi_l\|_{H^1}^2 < \infty, \quad \sum \lambda_l \int x^2|\psi_l(x)|^2\, dx < \infty\}. \quad (2.3)$$

We consider the problem of minimizing $\mathcal{E}(\Psi)$ in the space $\mathbb{Y}$ subject to the countably many constraints $\|\psi_l\|_{L^2} = 1$, $l = 1, 2, \ldots$ Solutions to this minimization problem satisfy the associated Euler-Lagrange equations, which are exactly the system (1.9-10). We now formulate our main result.

Theorem 2. *The energy functional $\mathcal{E}(\Psi)$ is bounded below on the subset of $\mathbb{Y}$ where $\|\psi_l\|_{L^2} = 1$, $l = 1, 2, \dots,$ and the minimum is assumed. The functions ψ_l which minimize $\mathcal{E}$ satisfy (1.9-10) in t he distributional sense, and the E_l are the Lagrange multipliers which arise from the constrained minimization.*

Proof. **1.** We first establish energy bounds from below. By the Cauchy-Schwarz inequality,

$$|\rho(x,y)|^2 \leq n(x)n(y),$$

hence

$$\begin{aligned}
&-\int\int \ln|x-y| \left(n(x)n(y) - |\rho(x,y)|^2\right) dxdy \\
&\geq -\int\int_{|x-y|\geq 1} \dots dxdy \\
&\geq -\int\int_{1\leq|x-y|<r} \dots dxdy - \frac{\ln r}{r^2}\int\int_{r\leq|x-y|} |x-y|^2 n(x)n(y)\, dxdy \\
&=: I + II,
\end{aligned}$$

where in the last step we chose $r > \sqrt{e}$. By the chosen normalization,

$$M := \sum \lambda_l \|\psi_l\|_{L^2}^2 = 1,$$

and we can estimate

$$I \geq -(\ln r)M^2 = -\ln r, \qquad II \geq -\frac{4\ln r}{r^2} M \sum \lambda_l \int |x|^2 |\psi_l(x)|^2\, dx.$$

Collecting these estimates, we find

$$\mathcal{E}(\Psi) \geq \frac{1}{4}\sum \lambda_l \int |\nabla\psi_l|^2\, dx - \frac{\ln r}{4\pi} + \left[\frac{\delta}{2}(1-\theta) - \frac{\ln r}{r^2\pi}\right] \sum_l \lambda_l \int |x|^2|\psi_l(x)|^2 dx.$$

The term $\frac{\delta}{2}(1-\theta) - \frac{\ln r}{r^2\pi}$ becomes positive for sufficiently large r (as a function of δ and θ) This proves that $\mathcal{E}(\Psi)$ is bounded below.

2. Let $\mathbb{Y}_c = \{\Psi \in \mathbb{Y};\ \|\psi_l\|_{L^2} = 1 \quad \forall l = 1, 2, \dots\}$. Choose a minimizing sequence $\{\Psi^n\}_{n\in\mathbb{N}} \subset \mathbb{Y}_c$ such that $\forall n, l$ $\|\psi_l^n\|_{L^2} = 1$ and $\mathcal{E}(\Psi^n) \to inf_{\mathbb{Y}_c}\mathcal{E}(\Psi)$ as $n \to \infty$. It follows from the bounds on $\mathcal{E}$ that there is a constant $C > 0$ such that

$$\sum_l \lambda_l \int |\nabla_x \psi_l^n|^2 dx < C, \qquad \sum_l \lambda_l \int |x|^2 |\psi_l^n(x)|^2\, dx < C. \tag{2.3}$$

Without restricting the generality, we may assume that the (fixed) constants λ_l are all strictly positive. Therefore, (2.3) implies

$$\int |\nabla_x \psi_l^n|^2\, dx < C/\lambda_l \quad \text{and} \quad \int |x|^2 |\psi_l^n(x)|^2 dx < C/\lambda_l$$

for all n, l. By compact embedding and a standard diagonal argument, we can extract a subsequence such that for all $l \in \mathbb{N}$ $\psi_l^n \to \psi_l$ as $n \to \infty$ in $L^2(\mathbb{R}^2)$. As the space $Y := \{\psi \in H^1(\mathbb{R}^2); \int |x|^2 |\psi(x)|^2 dx < \infty\}$ is continuously embedded in $L^p(\mathbb{R}^2)$ for all $p \in [2, \infty)$, we also can use Höl der's inequality to get strong convergence in all such L^p-spaces.

3. The minimizer $\Psi = \{\psi_l\}$ will satisfy the Euler-Lagra nge equations associated with our minimization problem if we can show that the nonlinear terms converge in the sense of distributions. To this end, let φ be a smooth test function, supported in $B_R(0) = \{x \in \mathbb{R}^2; \quad |x| \leq R\}$, and consider, say, the component of the self-consistent field $\int \ln|x - y||\psi_j^n(y)|^2 dy$. We abbreviate this as $U[\psi_j^n]$. Consider the nonlinear terms arising in the $l-$th equation. We write

$$\begin{aligned} &\int U[\psi_j^n]\psi_l^n(x)\varphi(x)dx - \int U[\psi_j]\psi_l(x)\varphi(x)dx \\ &= \int_{|x|\leq R} U[\psi_j^n]\left\{\psi_l^n(x) - \psi_l(x)\right\}\varphi(x)\, dx \\ &\quad + \int_{|x|\leq R} \left\{U[\psi_j^n] - U[\psi_j]\right\}\psi_l(x)\varphi(x)\, dx \\ &=: I_n + J_n. \end{aligned} \tag{2.4}$$

Further, abbreviating

$$K_j^n(x) := \int_{\mathbb{R}^2} |\ln|x - y||^q \left(|\psi_j^n(y)| + |\psi_j(y)|\right)^q dy$$

we estimate, using Hölder's inequality with $p \geq 2$ and $q = \frac{p}{p-1}$

$$|J_n| \leq \int_{|x|\leq R} K_j^n(x)^{1/q} \|\psi_j^n - \psi_j\|_{L^p} |\varphi(x)||\psi_l(x)|\, dx. \tag{2.5}$$

We now apply Hölder's inequality a second time, this time to $K_j^n(x)$, where we choose $t = \frac{2}{q} \geq 1$ and s such that $\frac{1}{s} + \frac{1}{t} = 1$. Then $s \in [2, \infty)$, and we get for $\epsilon > 0$

$$\begin{aligned} |K_j^n(x)| &\leq \int \frac{|\ln|x-y||^q (1+|y|)^\epsilon}{(1+|y|)^\epsilon} \left(|\psi_l^n(y)| + |\psi_l(y)|\right)^q \, dy \\ &\leq \left(\int \frac{|\ln|x-y||^{qs}}{(1+|y|)^{\epsilon s}} dy \right)^{1/s} \left(\int (1+|y|)^{\epsilon t} \left(|\psi_l^n(y)| + |\psi_l(y)|\right)^2 dy \right)^{1/t} . \end{aligned}$$

Choose $\epsilon t = 2$, i.e., $\epsilon = 2/t = q$. Then $\epsilon s = \frac{2q}{2-q}$, and the last line becomes

$$\left(\int \frac{|\ln|x-y||^{q\frac{2}{2-q}}}{(1+|y|)^{\frac{2q}{2-q}}} dy \right)^{2/(2-q)} \left(\int (1+|y|)^2 \left(|\psi_l^n(y)| + |\psi_l(y)|\right)^2 dy \right)^{q/2} .$$

The first factor in this last product is bounded as $|x| < R$ and $\frac{2q}{2-q} > 2$. The second factor is bounded because of the energy bounds . Since $|\varphi(x)| \cdot |\psi_j(x)|$ is in L^1, It follows using the dominated convergence theorem that J_n converges to zero. Similarly, one has that I_n converges to zero, and from this one easily concludes convergence of the nonlinear terms in the equation. This completes the proof of Theorem 2.

3. Three Dimensions. The method presented above generalizes with minor modifications to fermion clouds confined in three dimensions. There are only two changes.

We continue to assume that the exterior magnetic field is

$$\vec{A}(x) = \omega(-x_2, x_1, 0),$$

i.e., there is no x_3-component. The existence of a confined cloud in (quasi-) periodic motion is then only feasible if there is electric confinement in the x_3-direction, i.e., the external electric potential must have a part like Cx_3^2, with $C > 0$.

Otherwise, a particle cloud would disperse in this x_3-direction and approach vacuum as an asymptotic state (for the situation depicted here, this is physically reasonable, but mathematically just a conjecture; in Fermion systems without any confinement, decay results of this type were proved in [4].

With confinement, the energy functional corresponding to the three-dimensional case is

$$\begin{aligned}\mathcal{E}(\Psi) =& \frac{1}{4}\sum \lambda_l \int |\nabla \psi_l(x)|^2\, dx + \frac{1}{8\pi}\int\int \frac{1}{|x-y|}\left[n(x)n(y) - |\rho(x,y)|^2\right] dxdy \\ &+ \frac{\delta}{2}\int \left((1+\theta)x_1^2 + (1-\theta)x_2^2 + c_1 x_3^2\right) n(x)\, dx,\end{aligned}$$

with some $c_1 > 0$. It is immediate that $\mathcal{E}(\Psi)$ is bounded below (by 0) on $\mathbb{Y}_c$ as long as $0 \le \theta \le 1$.

Remark. As a mathematical curiosity with (probably) no physical implications, we point out that $\mathcal{E}(\Psi)$ remains bounded below

even in the fictitious case where the interparticle force is *attractive*, i.e., the case where the second term in the energy functional is

$$I_2 := -\frac{1}{8\pi}\int\int \frac{1}{|x-y|}\left[n(x)n(y) - |\rho(x,y)|^2\right] dxdy.$$

To this end, we estimate as on p. 357 in [5],

$$\begin{aligned}|I_2| \ge& -\frac{1}{8\pi}\int\int \frac{n(x)n(y)}{|x-y|} dxdy = \frac{1}{2}\int U(x)n(x)\, dx \\ =& \frac{1}{2}\int U(x)\Delta U(x)\, dx = -\frac{1}{2}\int |\nabla U(x)|^2 dx,\end{aligned}$$

and by Lemma 3.4 in [5] there is a constant $C > 0$ such that

$$\begin{aligned}\|\nabla U\|_{L^2}^2 \le& C\left(\sum \lambda_l \|\psi_l\|_{L^2}^2\right)^{3/2}\left(\sum \lambda_l \|\nabla\psi_l\|_{L^2}^2\right)^{1/2} \\ \le& C\left(\sum \lambda_l \|\nabla\psi_l\|_{L^2}^2\right)^{1/2} \\ \le& \frac{C}{\epsilon} + \epsilon\left(\sum \lambda_l \|\nabla\psi_l\|_{L^2}^2\right),\end{aligned}$$

where we have used that $\Psi \in \mathbb{Y}_c$. Choosing $\epsilon < 1/4$, the last term here can be absorbed in the first term in $\mathcal{E}(\Psi)$, and lower bounds on $\mathcal{E}(\Psi)$ follow.

For results on the time-dependent case involving attractive forces, we refer to [6] and [9].

The second part in our existence proof for the two-dimensional case now carries over without changes. Note that it is here that the confinement with respect to the x_3-direction becomes important; without it, we could not use compact embeddings.

There is also a difference in the Sobolev embedding quoted at the end of step 2. The continuous embedding now only holds for $2 \leq p \leq 6$ ($= \frac{2n}{n-2}$ with $n = 3$). The convergence argument for the nonlinear terms therefore requires more care.

Specifically, the estimates starting with (2.4) have to be modified as follows:

Let φ be a test function supported in $\{x \in \mathbb{R}^3; |x| \leq R\}$. To estimate

$$\int_{|x|\leq R} \int_y \frac{1}{|x-y|} \left(|\psi_j^n(y)|^2 - |\psi_j(y)|^2\right) \psi_l(x)\varphi(x) dy dx,$$

we break up the integration domain as

$$\int_{|x|\leq R} \int_{|x-y|<1} \ldots + \int_{|x|\leq R} \int_{|x-y|\geq 1} \ldots = I(n,l) + II(n,l).$$

Then, for $2 \leq p \leq 6$ and $1/q + 1/p = 1$, by Hölder's inequality

$$\begin{aligned} |I(n,l)| \leq & \|\psi_j^n - \psi_j\|_{L^p} \int_{|x|\leq R} \int_{|y-x|\leq 1} \frac{1}{|x-y|^q} \left|\psi_j^n + \psi_j\right|^q (y) dy |\psi_l(x)\varphi(x)| \, dx \\ \leq & C\|\psi_j^n - \psi_j\|_{L^p} \left(\int_{|y-x|\leq 1} \frac{1}{|x-y|^{qs}} dy\right)^{1/s} \left(\int \left|\psi_j^n + \psi_j\right|^{qr} (y) dy\right)^{1/r} \end{aligned}$$

where we need $qs < 3$ and $1 < r, s < \infty$, $\quad 1/r + 1/s = 1$. Choosing, say, $p = 6$, $q = 6/5$, $r = 5$ and $s = 5/4$ shows that $\lim_{n\to\infty} |I(n,l)| = 0$.

The convergence argument for $II(n,l)$ is even more straightforward. All we have to note is that

$$|II(n,l)| \leq C(\varphi, \psi_l) \|\psi_j^n - \psi_j\|_{L^2} \|\psi_j^n + \psi_j\|_{L^2}.$$

These estimates are sufficient for the convergence in the nonlinear terms in the minimization problem.

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