

HARTREE–FOCK COERCIVITY FOR TWISTED BILAYER GRAPHENE

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ABSTRACT. We study the minimisers of the Hartree–Fock functional for flat bands in the chiral model of twisted bilayer graphene [TKV19]. Our model is a continuous version of the discrete model considered by Becker, Lin and Stubbs [BLS25, SBL25] and the first result is a direct analogue of main theorems of those papers: at half filling of the flat band of multiplicity two, there are exactly two minimisers, obtained by occupying either one of the two sub-bands. (A more general version of this result, stressing its topological origins, was presented in [St26, §A.8].) The new contribution is the *strict* coercivity of the Hessian of the Hartree–Fock functional at the two minimisers. It is a consequence of the difference between the Chern numbers of the component bands and can be optimistically considered as a soft version of a “spectral gap”.

1. INTRODUCTION

The purpose of this note is to investigate a Hartree–Fock functional in the continuous model of interacting electrons in twisted bilayer graphene (TBG). The non-interacting part is based on Tarnopolsky, Kruchkov and Vishwanath’s [TKV19] chiral limit of the Bistritzer–MacDonald model [BiMa11], see §2 for a detailed review and references to mathematical results. The interacting model is the continuous version of the discrete model studied by Becker, Lin and Stubbs [BLS25, SBL25]. In these works, the discreteness came from considering supercells (large tori) and the consequent discretisation of quasi-momenta. Here we follow [St26] and work on $\mathbb{R}^2$ (rather than supercells) with continuous quasi-momenta. We refer to that appendix for a detailed presentation of this theory.

We now briefly describe the resulting Hartree–Fock problem. At a simple magic angle (see (2.10)), the Hamiltonian $H(\alpha)$ reviewed in §2 has a flat band of multiplicity two, described by a rank-two Bloch bundle $E = E_+ \oplus E_-$. To study the behavior of this system, we take the strong coupling approach and project the electrons-electron interactions to the flat bands (see Ledwith, Khalaf, Vishwanath [LKV21] for a review). We use the average subtraction scheme which determines a one-body subtraction term P_{sub} – see [St26, (A.8.10)]. Thus the effective one-body Hamiltonian and the corresponding many-electron Hamiltonian are, respectively,

$$P := H(\alpha) - P_{\text{sub}}, \quad \hat{P} + \mathbb{V} = \hat{H}(\alpha) + \mathbb{V} - \hat{P}_{\text{sub}},$$

where $\mathbb{V}$ is the second quantisation of the interaction term described in [St26, §A.6, §A.7]. (We avoid $\hat{V}$ used there, not to confuse $\mathbb{V}$ with the Fourier transform of V .) The subtraction $\hat{P}_{\text{sub}}$ is meant to remove interactions already incorporated in the one-body Hamiltonian. While minimizing the many-electron Hamiltonian is a formidable problem, it was observed in the physics literature – see Vafeek, Kang [KV19], Bultinck, Khalaf, Liu, Chatterjee, Vishwanath,

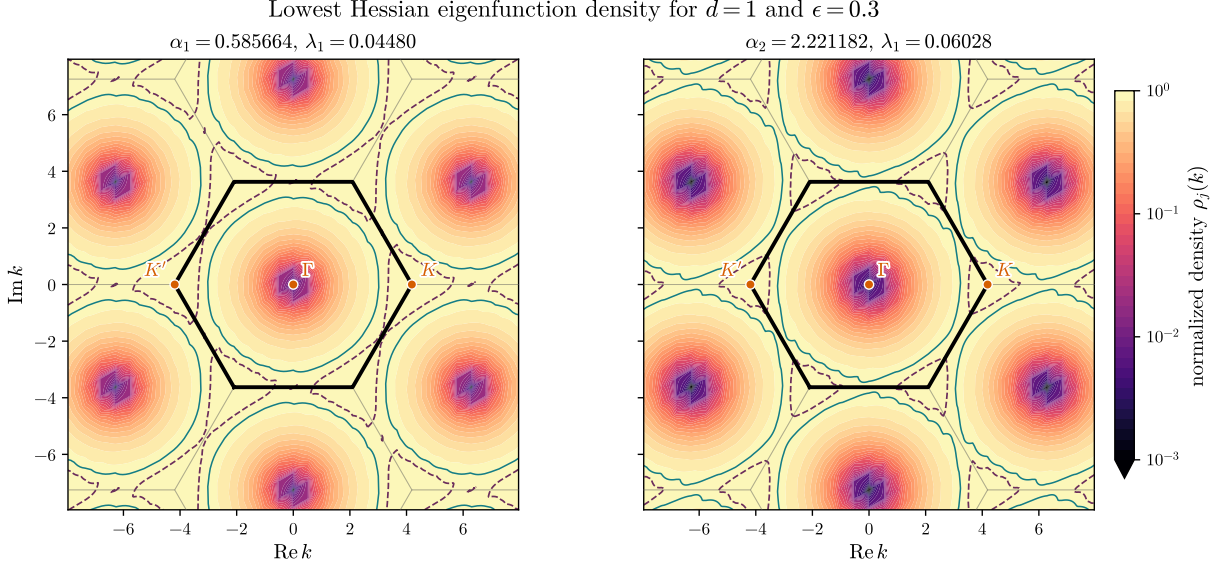


FIGURE 1. Numerically computed lowest eigenfunctions, ψ_1 (with the eigenvalues λ_1 determining the constants in (1.2)) for the first two magic angles of [TKV19]: the plot shows the log of the normalised density, $\rho_j(k) := |\psi_1(k)|^2 / \max_q |\psi_1(q)|^2$, for α_j , $j = 1, 2$. The parameters in (1.1) are $d = 1$ and $\epsilon = 0.3$. The vanishing at $\Gamma = 0$ follows from basic symmetries. This figure and Figure 2 were produced, on request, by ChatGPT 5.6.

and Zaletel [B*20], Bernevig, Song, Regnault, and Lian [Ber*21] – that the choice of average subtraction produces mathematically clean results. We refer to [St26, §A.8, (8.8)–(8.10)] for its mathematical formulation and to the references above for its motivation and use in interacting models of TBG.

A standard physical example of the interaction is the double-gate screened Coulomb interaction, whose Fourier transform is

$$\widehat{V}(\eta) = (2\pi/\epsilon) \tanh(\tfrac{1}{2}d|\eta|)/|\eta|, \quad \epsilon, d > 0, \quad (1.1)$$

which is bounded at $\eta = 0$ and is $\mathcal{O}(|\eta|^{-1})$ at infinity; see [BLS25, (2.23)] and [St26, (A.8.26)].

For a periodic one-particle density matrix γ , the Hartree–Fock energy per fundamental cell is

$$E_{\text{HF}}^\Lambda(\gamma) = \text{tr}_\Lambda(P\gamma) + \frac{1}{2} \int_\Omega \int_{\mathbb{R}^2} V(x-y) (\rho_\gamma(x)\rho_\gamma(y) - \text{tr}(\gamma(x,y)\gamma(y,x))) \, dy \, dx,$$

where $\rho_\gamma(x) := \text{tr} \gamma(x, x)$, Ω is a fundamental cell of Λ , and tr_Λ denotes trace per cell (see [St26, (8.1)–(8.3)]). After restriction to the flat band and the above subtraction, this becomes, up to irrelevant constants, the functional $E_{\text{H}}(\Pi) + E_{\text{X}}(\Pi)$ described in (3.12).

The flat band has rank two, and a translation-invariant Slater state is described in Bloch variables by a measurable field of orthogonal projections $\Pi(k) : E_k \rightarrow E_k$. We impose an

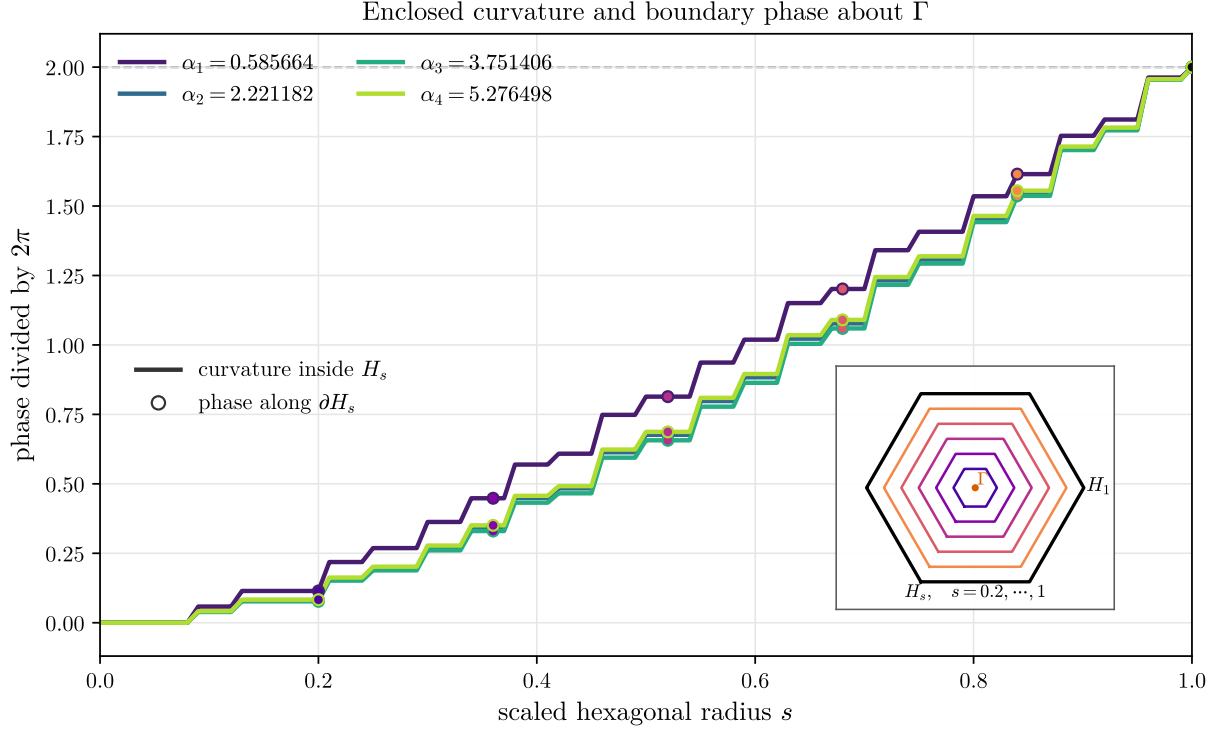


FIGURE 2. Curvature of the tangent line bundle at Π_+ , $E_- \otimes E_+^*$ (φ in (1.2) are essentially sections of it), equipped with its natural connection, for the first four positive magic parameters. Writing $H_s = sH_1$ where H_1 is the fundamental hexagon centred at Γ , the solid curves show the curvature enclosed by H_s (divided by 2π), and the circles, the corresponding continuously lifted phase along ∂H_s . Since $c_1(E_- \otimes E_+^*) = 2$, all four profiles have the common endpoint 2. Their intermediate shapes do however depend visibly on α , with the first magic parameter being the most distinct.

average half-filling condition:

$$\Pi(k)^2 = \Pi(k) = \Pi(k)^*, \quad |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}/\Lambda^*} \text{tr } \Pi(k) dk = 1.$$

The usual uniform half-filling condition $\text{tr } \Pi(k) = 1$ almost everywhere is a special case. Allowing the more general condition above is useful in the continuous setting and is discussed further in §3.2; see also [St26, §A.8] and [SBL25].

Our first result, stated precisely as Theorem 1, says that the only minimisers in this larger class are

$$\Pi = \Pi_+ \quad \text{and} \quad \Pi = \Pi_-,$$

the projections obtained by filling one of the two component flat bands. In particular, the minimisers are uniformly half-filled even though uniformity is not assumed. This is the continuous counterpart of the results of [BLS25, SBL25]. Its topological version in [St26,

Theorem 8.1] applies more generally to a transfer-invariant splitting into line bundles with different Chern numbers.

The new result of this note concerns stability of these minimisers. On the Hilbert manifold of rank-one projection fields, Theorem 2 gives, at either minimiser, the strict coercive estimate

$$\text{Hess}_{\Pi_{\pm}} E_{\text{HF}}(\varphi, \varphi) \geq c \int_{\mathbb{C}/\Lambda^*} |\varphi(k)|^2 dk, \quad c > 0. \quad (1.2)$$

The mechanism is topological: the component line bundles have different Chern numbers, which rules out a nonzero null direction for the Hessian. This can be viewed as a mean-field, or “soft”, analogue of a spectral gap, though we insist that it is not a statement about the spectral gap of the many-body Hamiltonian.

Figure 1 illustrates (1.2) numerically. It displays the lowest Hessian mode for the first two magic parameters: its eigenvalue, λ_1 , measures the weakest neutral variation away from the minimiser, while its density shows where that variation is concentrated in quasi-momentum space. Figure 2 displays the curvature of the tangent line bundle (the space where φ in (1.2) live) for the first four magic parameters, separating its topologically fixed total from its alpha dependent distribution.

We conclude this introduction with additional pointers to the literature. The positivity of the constrained Hartree–Fock Hessian is the usual stability condition for a Hartree–Fock state. In physics, Thouless [Th60] related this condition to the stability of collective modes in the random-phase approximation. Quantitative coercivity estimates appear to be much less common, and rigorous many-body gap results derived from such estimates seem rarer still. In the reduced Hartree–Fock model for defects in an insulating crystal, Cancès, Deleurence and Lewin [CDL08] obtained a global coercive bound from convexity and an assumed one-particle band gap. For the full Hartree–Fock functional of a weakly interacting Fermi gas on a finite torus, Benedikter, Nam, Porta, Schlein and Seiringer [Ben*21, Appendix A] proved a global coercive bound using a discrete kinetic gap. In the present flat-band problem the projected one-body energy is constant and supplies no such mechanism: the absence of zero modes, and hence coercivity, follows instead from the mismatch of the Chern numbers of the two component bands. To our knowledge, this topological mechanism for Hartree–Fock stability is new. Different notions of gap should also be kept separate. Bach, Lieb, Loss and Solovej [B*94] proved strict separation of occupied and unoccupied levels of the self-consistent Fock operator for finite systems, while [BLS25] establishes a charge gap for adding or removing an electron in the discrete flat-band model. Instead, the result here controls neutral orbital variations at fixed filling and does not by itself give a spectral gap above the ground-state sector of the many-electron Hamiltonian.

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2. REVIEW OF THE CHIRAL MODEL OF TBG

In this section we review the chiral Bistritzer–MacDonald Hamiltonian [BiMa11] studied in [TKV19]. For mathematical accounts of its properties see [Zw24, §2] and [BeZw24, §2.1] and references given there. To introduce the model we consider the lattice governing its symmetries:

$$\Lambda := \mathbb{Z} \oplus \omega \mathbb{Z}, \quad \omega := e^{2\pi i/3}, \quad \Lambda^* = \frac{4\pi i}{\sqrt{3}} \Lambda, \quad K = \frac{4}{3}\pi, \quad \langle z, w \rangle := \operatorname{Re}(z\bar{w}).$$

Here Λ^* is the dual (reciprocal) lattice and K is a point of high symmetry: $\omega K \equiv K \pmod{\Lambda^*}$. Let Ω^* be a fundamental cell of Λ^* .

In the coordinates of [Zw24, (2.2)–(2.3)] (see §2.1 there for the relation to other coordinate descriptions), the Hamiltonian $H(\alpha) : H^1(\mathbb{C}; \mathbb{C}^4) \rightarrow L^2(\mathbb{C}; \mathbb{C}^4)$ is given by

$$H(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* \\ D(\alpha) & 0 \end{pmatrix}, \quad D(\alpha) := \begin{pmatrix} 2D_{\bar{z}} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar{z}} \end{pmatrix}, \quad (2.1)$$

where $2D_{\bar{z}} = (\partial_{x_1} + i\partial_{x_2})/i$, $z = x_1 + ix_2$.

The dimensionless constant $\alpha \in \mathbb{C}$ is proportional to the inverse twisting angle and the potential, modelling tunnelling AB'/BA' sites is assumed to satisfy

$$U(z + \gamma) = e^{i\langle \gamma, K \rangle} U(z), \quad U(\omega z) = \omega U(z), \quad \overline{U(\bar{z})} = -U(-z), \quad \gamma \in \Lambda. \quad (2.2)$$

The specific Bistritzer–MacDonald potential [BiMa11] in this normalisation is given by

$$U_{\text{BM}}(z) = -\frac{4\pi i}{3} \sum_{\ell=0}^2 \omega^\ell e^{i\langle z, \omega^\ell K \rangle}. \quad (2.3)$$

We next recall the twisted periodicity and the modified Bloch transform – see [BeZw24, §2.1] and [Zw24, §3.1]. For $u \in L^2_{\text{loc}}(\mathbb{C}; \mathbb{C}^2)$ and $\gamma \in \Lambda$, define

$$L_\gamma u(z) := \begin{pmatrix} e^{i\langle \gamma, K \rangle} & 0 \\ 0 & e^{-i\langle \gamma, K \rangle} \end{pmatrix} u(z + \gamma), \quad \mathcal{L}_\gamma := \begin{pmatrix} L_\gamma & 0 \\ 0 & L_\gamma \end{pmatrix} \quad (2.4)$$

on $L^2_{\text{loc}}(\mathbb{C}; \mathbb{C}^4)$. We use the twisted periodic spaces

$$\begin{aligned} L_k^2(\mathbb{C}; \mathbb{C}^2) &:= \{u \in L^2_{\text{loc}}(\mathbb{C}; \mathbb{C}^2) : L_\gamma u = e^{i\langle k, \gamma \rangle} u, \gamma \in \Lambda\}, \\ L_k^2(\mathbb{C}; \mathbb{C}^4) &:= \{u \in L^2_{\text{loc}}(\mathbb{C}; \mathbb{C}^4) : \mathcal{L}_\gamma u = e^{i\langle k, \gamma \rangle} u, \gamma \in \Lambda\}, \end{aligned} \quad (2.5)$$

with norms taken over a fundamental cell of Λ . We also put $H_k^1 := H^1_{\text{loc}} \cap L_k^2$. These spaces depend only on $[k] \in \mathbb{C}/\Lambda^*$.

The modified Bloch transform is given, initially for Schwartz functions, by

$$\mathcal{B}f(k, z) := |\mathbb{C}/\Lambda^*|^{-1/2} \sum_{\gamma \in \Lambda} e^{i\langle z + \gamma, k \rangle} \mathcal{L}_\gamma f(z). \quad (2.6)$$

It satisfies

$$\mathcal{L}_\gamma \mathcal{B}f(k, \bullet) = \mathcal{B}f(k, \bullet), \quad \mathcal{B}f(k + p, z) = e^{i\langle z, p \rangle} \mathcal{B}f(k, z), \quad p \in \Lambda^*. \quad (2.7)$$

As in [TaZw26, §5.2], $\mathcal{B}$ extends to a unitary map

$$\mathcal{B} : L^2(\mathbb{C}; \mathbb{C}^4) \longrightarrow L^2(\mathbb{C}/\Lambda^*; V),$$

where the parent bundle (see [TaZw26, §9.1], [St26, §A.7]) is

$$\begin{aligned} V &:= (\mathbb{C} \times L_0^2(\mathbb{C}; \mathbb{C}^4)) / \sim, \quad (k, u) \sim (k + p, \tau(p)u), \\ [\tau(p)u](z) &:= e^{i\langle z, p \rangle} u(z), \quad p \in \Lambda^*. \end{aligned} \quad (2.8)$$

The chiral grading gives

$$V = V_+ \oplus V_-, \quad V_{\pm} := (\mathbb{C} \times L_0^2(\mathbb{C}; \mathbb{C}^2)) / \sim.$$

On the modified Bloch side we consider $H_k(\alpha)\mathcal{B}u(z, k) = (\mathcal{B}H(\alpha)u)(z, k)$, where

$$H_k(\alpha) = \begin{pmatrix} 0 & D(\alpha)^* + \bar{k} \\ D(\alpha) + k & 0 \end{pmatrix}, \quad D(\alpha) + k : H_0^1(\mathbb{C}; \mathbb{C}^2) \longrightarrow L_0^2(\mathbb{C}; \mathbb{C}^2). \quad (2.9)$$

The eigenvalues of $H_k(\alpha)$ are symmetric with respect to the origin and we write them as

$$\dots \leq -E_2(\alpha, k) \leq -E_1(\alpha, k) \leq 0 \leq E_1(\alpha, k) \leq E_2(\alpha, k) \leq \dots$$

A parameter α is *magic* if $E_1(\alpha, k) = 0$ for every k , and its chiral multiplicity is

$$m(\alpha) := \min\{j > 0 : \max_{k \in \mathbb{C}/\Lambda^*} E_{j+1}(\alpha, k) > 0\}. \quad (2.10)$$

(We remark that $E_1(\pm K, \alpha) = 0$ for all α and the positivity condition can be replaced by the existence of $k \neq \pm K + \Lambda^*$ such that $E_{j+1}(\alpha, k) = 0$ – see [BHZ25, Theorem 1].)

For a magic α , [BHZ26, Theorem 1] shows that, for every k ,

$$m(\alpha) = \dim \ker(D(\alpha) + k), \quad \dim \ker H_k(\alpha) = 2m(\alpha).$$

Thus a magic angle is called *simple* when $m(\alpha) = 1$. In that case, the corresponding flat band of the full Hamiltonian has multiplicity two. Magic angle multiplicities and their restrictions are studied in [BHZ26, IN25]. For the potential (2.3), Watson and Luskin [WaLu21] proved the existence of a real magic parameter in $(0.57, 0.61)$. Becker, Humbert and Zworski [BHZ23, Theorem 3] gave a different proof, locating the smallest positive magic parameter in $(0.583, 0.589)$ and proving that it is *simple*. In particular, the simple-magic-angle hypothesis used below is non-empty.

At a simple magic angle α , in the notation of [BeZw24],

$$\ker_{H_0^1}(D(\alpha) + k) = \mathbb{C}u(k), \quad \ker_{H_0^1}(D(\alpha)^* + \bar{k}) = \mathbb{C}u^*(k). \quad (2.11)$$

These kernels define smooth line subbundles $E_+ \subset V_+$ and $E_- \subset V_-$, with orthogonal projections

$$\Pi_{\pm}(k) : V_{\pm, k} \longrightarrow E_{\pm, k}. \quad (2.12)$$

We also put

$$\Pi_E(k) : V_k \longrightarrow E_k := E_{+, k} \oplus E_{-, k}, \quad \Pi_E(k) = \begin{pmatrix} \Pi_+(k) & 0 \\ 0 & \Pi_-(k) \end{pmatrix}. \quad (2.13)$$

The splitting $E = E_+ \oplus E_-$ is canonical. Moreover,

$$c_1(E_+) = -1, \quad c_1(E_-) = 1; \quad (2.14)$$

see [BHZ25, Theorem 4]. Hence $c_1(E) = 0$, and E is a trivial rank-two bundle over $\mathbb{C}/\Lambda^*$, although we do not choose a trivialisation until Section 4.

The chiral and antiunitary symmetries, respectively (see [BeZw24, (2.9),(2.10)]), give

$$u^*(k) = \mathcal{Q}u(k), \quad u(-k) = \rho(k)\mathcal{H}u(k), \quad |\rho(k)| = 1. \quad (2.15)$$

In particular, if $M_p v(z) = e^{i\langle p, z \rangle} v(z)$ and $A_k(p) := \langle u(k), M_p u(k) \rangle$, then

$$A_{-k}(p) = \overline{A_k(p)}. \quad (2.16)$$

We will use (2.14) in the topological part of the proofs below and (2.16) to verify a neutrality identity (3.19) needed to establish existence and uniqueness of minimisers (see Theorem 1).

3. MANY BODY INTERACTION PROJECTED TO THE FLAT BAND

3.1. Interaction projected to the flat band. We recall from [St26, §A.7] that the interaction for the N -body system is described using the multiplication operator M_η ,

$$M_\eta u(x) := e^{i\langle x, \eta \rangle} u(x) \quad (3.1)$$

projected to the flat band. We first describe it on the modified Bloch transform side. For $k \in \Omega^*$, denote the chosen representative of $[k - \eta] \in \mathbb{C}/\Lambda^*$ by $k_\eta \in \Omega^*$, and write

$$k - \eta = k_\eta + p_\eta(k), \quad p_\eta(k) \in \Lambda^*. \quad (3.2)$$

Multiplication by $e^{i\langle \eta, x \rangle}$ changes $e^{-i\langle k, x \rangle} u(x)$ into $e^{-i\langle k - \eta, x \rangle} u(x)$. As in [St26, §A.7] It induces the intrinsic parent-bundle map

$$T_\eta(k) : V_k \longrightarrow V_{k_\eta}, \quad T_\eta(k)[k, u] := [k - \eta, u]. \quad (3.3)$$

In the representatives chosen in (3.2), $T_\eta(k)[k, u] = [k_\eta, e^{-i\langle p_\eta(k), x \rangle} u]$, or equivalently,

$$(\mathcal{B}M_\eta\mathcal{B}^{-1}s)(k_\eta) = T_\eta(k)s(k).$$

By (2.13), the smooth subbundle $E_+ \oplus E_- \subset V$ defines the orthogonal projection

$$\Pi_E := \mathcal{B}^{-1}\Pi(\bullet)\mathcal{B}, \quad (\Pi(\bullet)s)(k) := \Pi(k)s(k).$$

The Bloch representative of $\Pi_E M_\eta \Pi_E$ is

$$L_\eta := \mathcal{B}\Pi_E M_\eta \Pi_E \mathcal{B}^{-1} : L^2(\mathbb{C}/\Lambda^*; E) \longrightarrow L^2(\mathbb{C}/\Lambda^*; E). \quad (3.4)$$

Explicitly, for $s \in L^2(\mathbb{C}/\Lambda^*; E)$, we write L_η in terms of a bundle morphism:

$$(L_\eta s)(k_\eta) = \Lambda_\eta(k)s(k), \quad \Lambda_\eta(k) := \Pi(k_\eta)T_\eta(k)|_{E_k} : E_k \longrightarrow E_{k_\eta}. \quad (3.5)$$

A coordinate expression in a fundamental cell is given by $\Lambda_\eta(k) = \Pi(k_\eta)e^{-i\langle p_\eta(k), x \rangle}|_{E_k}$. We recall the properties of $\Lambda_\eta(k)$:

$$\Lambda_0(k) = I_{E_k}, \quad \Lambda_{-\eta}(k_\eta) = \Lambda_\eta(k)^*, \quad \|\Lambda_\eta(k)\| \leq 1. \quad (3.6)$$

We also note that $\Lambda_\eta(k)$ depends smoothly on (k, η) in the bundle sense. Put

$$\kappa(k, \eta) := [k - \eta], \quad \pi_1(k, \eta) := k.$$

Then the maps $T_\eta(k)$ in (3.3) define a smooth bundle isomorphism $T : \pi_1^* V \longrightarrow \kappa^* V$. (This is immediate from the quotient construction of V , since on the covering space T is induced by $(k, \eta, u) \longmapsto (k - \eta, u)$.) Since $E \subset V$ and the orthogonal projections $\Pi_E(k)$ are smooth, (3.5) defines a smooth bundle morphism

$$\Lambda : \pi_1^* E \longrightarrow \kappa^* E. \quad (3.7)$$

A representative k_η in a fixed fundamental cell need not depend smoothly on (k, η) but this is only an artefact of the choice of representatives.

After applying $\mathcal{B} \otimes \mathcal{B}$, the interaction restricted to the Bloch subbundle E is

$$\begin{aligned} V_E &:= (\mathcal{B} \otimes \mathcal{B})(\Pi_E \otimes \Pi_E)V(\Pi_E \otimes \Pi_E)(\mathcal{B}^{-1} \otimes \mathcal{B}^{-1}) \\ &= \frac{1}{(2\pi)^d} \int_{\mathbb{C}} \hat{V}(\eta) L_\eta \otimes L_{-\eta} d\eta, \end{aligned} \quad (3.8)$$

where $\hat{V}(\eta) := \int_{\mathbb{R}^2} V(x) e^{-i\langle \eta, x \rangle} dx$ is the Fourier transform of V – see [St26, (7.14), (7.48)].

Using the canonical splitting (2.13) the above discussion applies to E replaced by line bundles $E_\pm$ and in particular we have

$$\Lambda_\eta(k) = \begin{pmatrix} \Lambda_{+, \eta}(k) & 0 \\ 0 & \Lambda_{-, \eta}(k) \end{pmatrix}. \quad (3.9)$$

3.2. Hartree–Fock functional for flat bands at half-filling. We follow [St26, §A.8] and take potentials satisfying

$$\begin{aligned} V &\in C(\mathbb{R}^2), \quad \hat{V}(\eta) \geq 0, \quad \hat{V}(\eta) = \mathcal{O}(|\eta|^{-1}), \\ \hat{V}(\eta) &> 0 \quad \text{for } |\eta| < \varepsilon_V, \quad \varepsilon_V > 0. \end{aligned} \quad (3.10)$$

However, we now assume a (possibly) *non-uniform* half-filling (as was also possible in [St26, §A.8] – see [SBL25] for the discrete case), that is a measurable projection valued function,

$$\Pi(k)^2 = \Pi(k) = \Pi(k)^*, \quad |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}/\Lambda^*} \text{tr } \Pi(k) = 1. \quad (3.11)$$

This is a *half-filling* as the projection to the full bundle satisfies $\text{tr } \Pi_E(k) = 2$.

Following the physics literature (see [Ber*21, (3), (4), and (C8)–(C12)], [F*23, §I.3, §IV.2, (15)–(17)] and references given there) we consider the Hartree–Fock functional for a subtraction scheme taking into account interaction “double counting”. Its mathematical description is given in greater generality in [St26, (3.21)–(3.23)] and here we recall from [St26, (3.31), (3.32)] that we are minimising

$$\Pi \mapsto E_H(\Pi) + E_X(\Pi), \quad (3.12)$$

where, putting

$$Q(k) := 2\Pi(k) - I_{E_k}, \quad Q(k)^* = Q(k), \quad Q(k)^2 = I_{E_k}, \quad |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}/\Lambda^*} \text{tr } Q(k) dk = 0. \quad (3.13)$$

we have

$$E_H(\Pi) := \frac{1}{4(2\pi)^2} |\mathbb{C}/\Lambda^*|^{-1} \sum_{p \in \Lambda^*} \hat{V}(p) \left| \int_{\mathbb{C}/\Lambda^*} \text{tr}(\Lambda_p(k) Q(k)) dk \right|^2,$$

$$E_X(\Pi) := -\frac{1}{4(2\pi)^2} |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}} \hat{V}(\eta) \int_{\mathbb{C}/\Lambda^*} \text{tr}(\Lambda_\eta(k) Q(k) \Lambda_\eta(k)^* Q(k_\eta)) dk d\eta.$$

The first theorem is an adaptation of the results of [BLS25, SBL25] (for simple magic angles) to the continuous setting. A more general version formulated using discrepancy of Chern numbers of $E_\pm$ was presented in [St26, §A.8] for uniform half-filling. For reader's convenience, we present a complete argument in the case of the chiral model of TBG:

Theorem 1. *Assume that $\hat{V}$ satisfies (3.10). If $E = E_+ \oplus E_-$ where $E_\pm$ are the flat band line bundles associated to a simple magic angle, the only measurable fields (3.11) minimising $\Pi \rightarrow E_H(\Pi) + E_X(\Pi)$ (see (3.12)) are $\Pi = \Pi_+$ and $\Pi = \Pi_-$, where $\Pi_\pm$ are the projection onto $E_\pm$.*

Proof. We start with the elementary identity, used earlier in this context in [SBL25]:

$$\text{tr}(\Lambda Q \Lambda^* Q') = \|\Lambda\|_{\mathcal{L}_2}^2 - \frac{1}{2} \|Q' \Lambda - \Lambda Q\|_{\mathcal{L}_2}^2 \quad (3.14)$$

which holds whenever Q, Q' are self-adjoint involutions. Hence

$$E_X(\Pi) = E_X^{\min} + \frac{1}{8(2\pi)^2} |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}} \hat{V}(\eta) \int_{\mathbb{C}/\Lambda^*} \|Q(k_\eta) \Lambda_\eta(k) - \Lambda_\eta(k) Q(k)\|_{\mathcal{L}_2}^2 dk d\eta, \quad (3.15)$$

where

$$E_X^{\min} := -\frac{1}{4(2\pi)^2} |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}} \hat{V}(\eta) \int_{\mathbb{C}/\Lambda^*} \|\Lambda_\eta(k)\|_{\mathcal{L}_2}^2 dk d\eta \quad (3.16)$$

is independent of Π . All the quantities above are finite. To see this, write $\eta = q + p$, where q belongs to a fixed fundamental domain of Λ^* and $p \in \Lambda^*$. In local smooth orthonormal frames of E_k and E_{k_q} , the matrix entries of $\Lambda_{q+p}(k)$ have the form

$$\int_{\mathbb{C}/\Lambda} e^{-i\langle p, x \rangle} a_{ij}(k, q, x) dx,$$

where a_{ij} is smooth and periodic in x . Since $\mathbb{C}/\Lambda^*$ is compact, finitely many such frames suffice, and all x -derivatives of the corresponding functions a_{ij} are bounded uniformly in (k, q) . Repeated integration by parts therefore gives, for every N ,

$$\sup_{k, q} \|\Lambda_{q+p}(k)\|_{\mathcal{L}_2(E_k, E_{k_q})} \leq C_N \langle p \rangle^{-N}. \quad (3.17)$$

Together with $\hat{V}(\eta) = \mathcal{O}(\langle \eta \rangle^{-1})$, this proves the required absolute convergence.

Let $Q_\pm := 2\Pi_\pm - I_E$. By (3.9), $Q_\pm$ commutes with the bundle morphisms:

$$Q_\pm(k_\eta) \Lambda_\eta(k) = \Lambda_\eta(k) Q_\pm(k). \quad (3.18)$$

We now check their Hartree energy. For $p \in \Lambda^*$, (2.15)–(2.16) give

$$\Lambda_p(k) = \begin{pmatrix} A_k(p) & 0 \\ 0 & A_k(p) \end{pmatrix}, \quad Q_+(k) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and therefore $\text{tr}(\Lambda_p(-k)Q_+(-k)) = -\text{tr}(\Lambda_p(k)Q_+(k))$. The change of variables $k \mapsto -k$ shows that

$$\int_{\mathbb{C}/\Lambda^*} \text{tr}(\Lambda_p(k)Q_+(k)) dk = 0. \quad (3.19)$$

Since $Q_- = -Q_+$, the same holds for Q_- . Thus $E_H(\Pi_\pm) = 0$, and (3.18) and (3.15) show that both Π_+ and Π_- have energy $E_X^{\min}$.

Conversely, $E_H \geq 0$ and the second term in (3.15) is nonnegative. Hence every minimizer must make both terms vanish.

We now adapt the proof of [St26, Theorem 8.1] to the non-uniform filling. Hence, suppose that Q is a minimizer of the Hartree-Fock energy. Since, $\hat{V} > 0$ on $|\eta| < \varepsilon_V$, Fubini's theorem gives

$$Q(k_\eta)\Lambda_\eta(k) = \Lambda_\eta(k)Q(k) \quad (3.20)$$

for almost every (k, η) with $|\eta| < \varepsilon_V$.

We next replace the merely measurable Q by a smooth representative. Since $\Lambda_0(k) = I_{E_k}$, smoothness and compactness give $\varepsilon_0 > 0$ such that

$$\Lambda_\eta(k)^* \Lambda_\eta(k) \geq \frac{1}{2} I_{E_k}, \quad |\eta| < \varepsilon_0. \quad (3.21)$$

Put $\varepsilon_* := \min(\varepsilon_V, \varepsilon_0)$ and choose $\chi \in C_c^\infty(B(0, \varepsilon_*))$, $\chi \geq 0$, with $\int \chi(\eta) d\eta = 1$. Then

$$\tilde{Q}(k) := \int \chi(\eta) \Lambda_\eta(k)^{-1} Q(k_\eta) \Lambda_\eta(k) d\eta \quad (3.22)$$

equals $Q(k)$ for almost every k , by (3.20), and is smooth. This follows in local trivializations, after the change of variables $k' = k_\eta$, since (3.22) is then the integral of the L^∞ field $Q(k')$ against a smooth compactly supported kernel (see (3.7)). From now on we use this smooth representative. The two sides of (3.20) are now smooth in (k, η) , so that the identity holds for every k and every $|\eta| < \varepsilon_*$.

We can therefore assume that $\Pi = (Q + I_E)/2$ is a smooth family of projections. Its rank is therefore constant on the connected torus $\mathbb{C}/\Lambda^*$. The non-uniform half-filling condition (3.11), or equivalently the last identity in (3.13), then forces this constant rank to be one. Hence

$$L := \text{Ran } \Pi \subset E_+ \oplus E_-$$

is a smooth line subbundle. By (2.14), $c_1(E_+) \neq c_1(E_-)$. Thus at some k_0 one has

$$L_{k_0} = E_{+,k_0} \quad \text{or} \quad L_{k_0} = E_{-,k_0}. \quad (3.23)$$

Indeed, otherwise the two bundle projections $L \rightarrow E_+$ and $L \rightarrow E_-$ would be nowhere zero, hence line-bundle isomorphisms, which would imply $c_1(E_+) = c_1(L) = c_1(E_-)$.

Finally, (3.20), (3.21), and (3.18) imply, for $|\eta| < \varepsilon_*$,

$$\Lambda_\eta(k)L_k = L_{k_\eta}, \quad \Lambda_\eta(k)E_{\pm,k} = E_{\pm,k_\eta}.$$

Either equality in (3.23) therefore propagates to a neighborhood. Its equality set is also closed, and the torus $\mathbb{C}/\Lambda^*$ is connected. Hence $L = E_+$ or $L = E_-$, that is, $\Pi = \Pi_+$ or $\Pi = \Pi_-$ almost everywhere. $\square$

4. STRICT COERCIVITY OF THE HARTREE-FOCK FUNCTIONAL

In this section we prove that the functional (3.12) has a strictly positive Hessian at the minimisers obtained in Theorem 1. Although that theorem allowed non-uniform filling, both minimisers have rank one at every k . We therefore consider the Hessian on the Hilbert manifold of rank-one projection fields. The proof of coercivity follows from analysing (3.14) and a simple topological argument.

4.1. **Tangent space.** For the purposes of this section, choose a unitary trivialisation

$$E \simeq (\mathbb{C}/\Lambda^*) \times \mathbb{C}^2.$$

The rank-one projection fields of H^2 regularity form a Hilbert manifold, identified in this trivialisation with $H^2(\mathbb{C}/\Lambda^*; \mathbb{S}^2)$ by

$$\Pi_f(k) = \frac{1}{2}(I + f(k) \cdot \sigma), \quad Q_f(k) := 2\Pi_f(k) - I = f(k) \cdot \sigma, \quad (4.1)$$

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices. We stress that the trivialisation is used only to write this formula. We also stress that H^2 could be replaced by H^r for any $r > 1$ (so that the resulting functions of k are continuous) but we fix a Hilbert space giving a natural manifold structure to the projections.

The canonical splitting

$$E = E_+ \oplus E_- \quad (4.2)$$

is *not* the fixed coordinate splitting of $\mathbb{C}^2$ in this trivialisation.

Let $f_+ \in \mathcal{M}$ correspond to Π_+ in the identification (4.1). Then $Q_+ = 2\Pi_+ - I = f_+ \cdot \sigma$. Since Π_+ is the projection onto E_+ , the $+1$ and -1 eigenspace bundles of Q_+ are E_+ and E_- , respectively. Thus the canonical splitting (4.2) is the eigenspace splitting of the generally non-constant matrix field $Q_+(k)$.

The tangent space at f_+ is

$$\begin{aligned} \mathcal{T}_+ &:= T_{f_+}(H^2(\mathbb{C}/\Lambda^*; \mathbb{S}^2)) = \{\varphi \in H^2(\mathbb{C}/\Lambda^*; \mathbb{R}^3) : \forall k \langle \varphi(k), f_+(k) \rangle_{\mathbb{R}^3} = 0\} \\ &= H^2(\mathbb{C}/\Lambda^*; f_+^* T\mathbb{S}^2). \end{aligned} \quad (4.3)$$

(Here $f_+^* T\mathbb{S}^2$ is the pullback for the tangent bundle $T\mathbb{S}^2 \rightarrow \mathbb{S}^2$ – see [TaZw26, (2.29)].) The orthogonality condition in (4.3) follows by differentiating $|f_t(k)|^2 = 1$. Conversely, every $\varphi \in \mathcal{T}_+$ is obtained by differentiating a C^2 curve in $t \mapsto f_t \in H^2(\mathbb{C}/\Lambda^*; \mathbb{S}^2)$, $f_0 = f_+$, at $t = 0$. We can take for instance,

$$f_t(k) = \frac{f_+(k) + t\varphi(k)}{(1 + t^2|\varphi(k)|^2)^{1/2}}. \quad (4.4)$$

For $\varphi \in \mathcal{T}_+$ put

$$X_\varphi(k) := \varphi(k) \cdot \sigma.$$

Then

$$X_\varphi^* = X_\varphi, \quad Q_+ X_\varphi + X_\varphi Q_+ = 0, \quad \|X_\varphi(k)\|_{\mathcal{L}_2}^2 = 2|\varphi(k)|^2. \quad (4.5)$$

The anticommutation identity in (4.5) says exactly that X_φ is off-diagonal with respect to the canonical splitting $E = E_+ \oplus E_-$. Indeed, since

$$\Pi_+ = \frac{1}{2}(I + Q_+), \quad \Pi_- = \frac{1}{2}(I - Q_+),$$

the identity $Q_+X_\varphi + X_\varphi Q_+ = 0$ and $Q_- = -Q_+$ give $\Pi_+X_\varphi\Pi_+ = \Pi_-X_\varphi\Pi_- = 0$. Consequently,

$$X_\varphi = \psi_\varphi + \psi_\varphi^*, \quad \psi_\varphi := \Pi_-X_\varphi\Pi_+ \in H^2(\mathbb{C}/\Lambda^*; \text{Hom}(E_+, E_-)).$$

Thus $f_+^*TS^2$ is identified, as a real rank-two bundle, with the underlying real bundle of $\text{Hom}(E_+, E_-)$. In a local unitary frame adapted to the canonical splitting, rather than in the fixed trivialisation used to define the Pauli matrices, this says simply that

$$Q_+(k) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad X_\varphi(k) = \begin{pmatrix} 0 & \overline{z_\varphi(k)} \\ z_\varphi(k) & 0 \end{pmatrix}.$$

The scalar z_φ is only a local coordinate; globally the lower-left entry is the section ψ_φ above.

4.2. The Hessian at the minimisers. We now prove coercivity on the L^2 completion of $\mathcal{T}_+$ in (4.3) $L^2(\mathbb{C}/\Lambda^*; f_+^*TS^2)$. For $\varphi \in \mathcal{T}_+$, choose a C^2 curve

$$t \longmapsto f_t \in H^2(\mathbb{C}/\Lambda^*; \mathbb{S}^2), \quad f_0 = f_+, \quad \partial_t f_t|_{t=0} = \varphi,$$

for instance the curve in (4.4). Using that we define the Hessian as the quadratic form

$$\text{Hess}_{\Pi_+} E_{\text{HF}}(\varphi, \varphi) := \left. \frac{d^2}{dt^2} \right|_{t=0} E_{\text{HF}}(\Pi_{f_t}), \quad \Pi_+ = \Pi_{f_+}. \quad (4.6)$$

As in finite dimensions the Hessian is independent of the choice of f_t as Π_{f_+} is critical for $E_{\text{HF}}(\Pi_{f_t})$. Our main result is the strict coercivity of this Hessian:

Theorem 2. *In the setting of Theorem 1, the Hessian of E_{HF} restricted to the rank-one Hilbert manifold at Π_+ extends from $\mathcal{T}_+$ to a bounded quadratic form on $\mathcal{H}_+$. There exists $c_+ > 0$ such that*

$$\text{Hess}_{\Pi_+} E_{\text{HF}}(\varphi, \varphi) \geq c_+ \int_{\mathbb{C}/\Lambda^*} |\varphi(k)|^2 dk, \quad \varphi \in \mathcal{H}_+ := L^2(\mathbb{C}/\Lambda^*; f_+^*TS^2). \quad (4.7)$$

The analogous statement holds at Π_- .

Proof. By (3.19), $E_{\text{H}}(\Pi_+) = 0$, while $E_{\text{H}} \geq 0$. Hence the second variation of E_{H} at Π_+ along the rank-one Hilbert manifold is nonnegative, and it is enough to prove a coercive lower bound for the exchange Hessian.

The square in (3.15) vanishes at Q_+ , and differentiation gives the following expression for (4.6):

$$\frac{1}{4(2\pi)^2} |\mathbb{C}/\Lambda^*|^{-1} \int_{\mathbb{C}} \widehat{V}(\eta) \int_{\mathbb{C}/\Lambda^*} \|X_\varphi(k_\eta)\Lambda_\eta(k) - \Lambda_\eta(k)X_\varphi(k)\|_{\mathcal{L}_2}^2 dk d\eta. \quad (4.8)$$

Thus the exchange Hessian has the same transfer-defect form as the positive part of the exchange energy. This is because that part of the energy is the square of an expression which is linear in Q and vanishes at the minimiser. The same estimates as in (3.17) show that the

right hand side of (4.8) extends to a bounded quadratic form on $\mathcal{H}_+ := L^2(\mathbb{C}/\Lambda^*; f_+^* T\mathbb{S}^2)$, and

$$\text{Hess}_{\Pi_+} E_{\text{HF}}(\varphi, \varphi) \geq \text{Hess}_{\Pi_+} E_X(\varphi, \varphi), \quad \varphi \in \mathcal{T}_+. \quad (4.9)$$

We recall from (3.21) that $\Lambda_\eta(k)^* \Lambda_\eta(k) \geq \frac{1}{2}I$, for $|\eta| < \varepsilon$. For those values, let

$$\Lambda_\eta(k) = U_\eta(k) S_\eta(k), \quad S_\eta(k) := (\Lambda_\eta(k)^* \Lambda_\eta(k))^{1/2}, \quad (4.10)$$

be its polar decomposition. Then $U_\eta(k) : E_k \rightarrow E_{k_\eta}$ is unitary and $S_\eta(k) \geq 2^{-1/2}I$. Since $\Lambda_\eta(k)$ preserves the canonical splitting, $S_\eta(k)$ preserves $E_{+,k}$ and $E_{-,k}$, while $U_\eta(k)$ maps these spaces unitarily onto E_{+,k_η} and E_{-,k_η} , respectively. Both factors depend smoothly on (k, η) .

The identity (3.18) at Q_+ and the polar decomposition give

$$Q_+(k_\eta) U_\eta(k) = U_\eta(k) Q_+(k).$$

Indeed, $S_\eta(k)$ commutes with $Q_+(k)$ and is invertible. Conjugation by $U_\eta(k)$ defines $R_\eta(k) \in SO(3)$ by

$$U_\eta(k)(v \cdot \sigma) U_\eta(k)^* = (R_\eta(k)v) \cdot \sigma, \quad v \in \mathbb{R}^3. \quad (4.11)$$

Since $Q_+(k) = f_+(k) \cdot \sigma$, the intertwining identity gives

$$R_\eta(k) f_+(k) = f_+(k_\eta).$$

Consequently,

$$R_\eta(k) : T_{f_+(k)} \mathbb{S}^2 \longrightarrow T_{f_+(k_\eta)} \mathbb{S}^2$$

is an isometry, depending smoothly on (k, η) , and $R_{-\eta}(k_\eta) = R_\eta(k)^{-1}$.

In particular, $U_\eta(k)^* X_{\varphi(k_\eta)} U_\eta(k) = X_{R_\eta(k)^{-1} \varphi(k_\eta)}$. Since $R_\eta(k)^{-1} \varphi(k_\eta)$ and $\varphi(k)$ both belong to $T_{f_+(k)} \mathbb{S}^2$, the two self-adjoint matrices

$$A := U_\eta(k)^* X_{\varphi(k_\eta)} U_\eta(k), \quad B := X_{\varphi(k)}$$

are off-diagonal with respect to the same canonical splitting $E_k = E_{+,k} \oplus E_{-,k}$.

We now use the following elementary Hilbert–Schmidt norm estimate. In a local frame adapted to this splitting, write $S = \text{diag}(s_+, s_-)$ and represent the off-diagonal self-adjoint matrices A, B by $a, b \in \mathbb{C}$. Then

$$\|AS - SB\|_{\mathcal{L}_2}^2 = 2s_+ s_- |a - b|^2 + (s_+ - s_-)^2 (|a|^2 + |b|^2),$$

and since $\|A - B\|_{\mathcal{L}_2}^2 = 2|a - b|^2$,

$$S \geq \gamma I \implies \|AS - SB\|_{\mathcal{L}_2} \geq \gamma \|A - B\|_{\mathcal{L}_2}. \quad (4.12)$$

(For related inequalities in greater generality, see for instance, [Bh97, Chapter VIII.3].)

Applying (4.12) with $S = S_\eta(k)$ and using (4.5), we obtain (note that (4.5) has a factor of 2)

$$\|X_\varphi(k_\eta) \Lambda_\eta(k) - \Lambda_\eta(k) X_\varphi(k)\|_{\mathcal{L}_2}^2 \geq |\varphi(k_\eta) - R_\eta(k) \varphi(k)|^2. \quad (4.13)$$

To analyse the right hand side, we define the unitary operator $\mathcal{U}_\eta$ on $\mathcal{H}_+$ by

$$(\mathcal{U}_\eta \varphi)(k_\eta) := R_\eta(k) \varphi(k). \quad (4.14)$$

The identity $\Lambda_{-\eta}(k_\eta) = \Lambda_\eta(k)^*$ and uniqueness of the polar decomposition give $\mathcal{U}_{-\eta} = \mathcal{U}_\eta^*$. Shrinking ε below the injectivity radius of the torus if necessary, choose an even function $\chi \in C_c^\infty(B(0, \varepsilon))$, $\chi \geq 0$, which is positive near 0, and put

$$q(\varphi) := \int_{\mathbb{C}} \chi(\eta) \|\mathcal{U}_\eta \varphi - \varphi\|_{\mathcal{H}_+}^2 d\eta. \quad (4.15)$$

It follows from (4.9), (4.8), and (4.13) that

$$\text{Hess}_{\Pi_+} E_{\text{HF}}(\varphi, \varphi) \geq c_0 q(\varphi) \quad (4.16)$$

for some $c_0 > 0$. It remains to prove that

$$q(\varphi) \geq c_1 \|\varphi\|_{\mathcal{H}_+}^2, \quad c_1 > 0. \quad (4.17)$$

For that we define

$$c_\chi := \int_{\mathbb{C}} \chi(\eta) d\eta > 0, \quad K_\chi := \int_{\mathbb{C}} \chi(\eta) \mathcal{U}_\eta d\eta : \mathcal{H}_+ \longrightarrow \mathcal{H}_+. \quad (4.18)$$

Since $\mathcal{U}_\eta$ is unitary and χ is even, $K_\chi = K_\chi^*$, $\|K_\chi\| \leq c_\chi$, and

$$q(\varphi) = 2c_\chi \|\varphi\|_{\mathcal{H}_+}^2 - 2 \text{Re} \langle K_\chi \varphi, \varphi \rangle_{\mathcal{H}_+}. \quad (4.19)$$

The operator K_χ is smoothing, hence compact. Indeed, after the change of variables $k' = k_\eta$, it is an integral operator with a smooth bundle kernel, since $(k, \eta) \mapsto R_\eta(k)$ is smooth and χ is smooth and supported in a sufficiently small neighborhood of 0.

Suppose that (4.17) were false. We could then find $\varphi_j \in \mathcal{H}_+$ such that

$$\|\varphi_j\|_{\mathcal{H}_+} = 1, \quad q(\varphi_j) \longrightarrow 0.$$

After passage to a subsequence, $\varphi_j \rightharpoonup \varphi$ weakly in $\mathcal{H}_+$, with $\|\varphi\|_{\mathcal{H}_+} \leq 1$. Compactness gives $K_\chi \varphi_j \rightarrow K_\chi \varphi$ strongly, and (4.19) therefore yields

$$\text{Re} \langle K_\chi \varphi, \varphi \rangle_{\mathcal{H}_+} = c_\chi.$$

Since $\|K_\chi\| \leq c_\chi$, this implies $\|\varphi\|_{\mathcal{H}_+} = 1$. Hence $\varphi_j \rightarrow \varphi$ strongly and $q(\varphi) = 0$.

The nonnegative operator $c_\chi I - K_\chi$ therefore annihilates φ . Since K_χ is smoothing, φ is smooth. From (4.15) and the fact that χ is positive near 0, we obtain

$$\varphi(k_\eta) = R_\eta(k) \varphi(k), \quad k \in \mathbb{C}/\Lambda^*, \quad |\eta| \ll 1. \quad (4.20)$$

The zero set of φ is consequently both open and closed. Since the torus is connected and $\|\varphi\|_{\mathcal{H}_+} = 1$, the section φ is nowhere zero. On the other hand,

$$f_+^* TS^2 \simeq \text{Hom}(E_+, E_-), \quad c_1(\text{Hom}(E_+, E_-)) = 2.$$

Thus $f_+^* TS^2$ has no nowhere-vanishing sections, which gives a contradiction. Hence (4.17) holds, and (4.16) proves (4.7).

The assertion at Π_- follows by interchanging E_+ and E_- . Equivalently, $Q_- = -Q_+$ and $f_- = -f_+$, so the same tangent planes and the same argument apply; the relevant complex line bundle is $\text{Hom}(E_-, E_+)$, whose Chern number is -2 . $\square$

Remark. Although only positivity of E_H was needed in the proof, its second variation at the two minimisers actually vanishes. Indeed, put

$$F_p(Q) := \int_{\mathbb{C}/\Lambda^*} \text{tr}(\Lambda_p(k)Q(k)) dk.$$

Then $F_p(Q_+) = 0$ by (3.19). If Q_t is a curve through Q_+ with $\partial_t Q_t|_{t=0} = X_\varphi$, then

$$\left. \frac{d}{dt} \right|_{t=0} F_p(Q_t) = \int_{\mathbb{C}/\Lambda^*} \text{tr}(\Lambda_p(k)X_\varphi(k)) dk = 0,$$

since $\Lambda_p(k)$ is diagonal and $X_\varphi(k)$ is off-diagonal with respect to $E_+ \oplus E_-$. Hence

$$\left. \frac{d^2}{dt^2} \right|_{t=0} |F_p(Q_t)|^2 = 0,$$

and consequently, using the same absolute convergence estimates as above,

$$\text{Hess}_{\Pi_+} E_H(\varphi, \varphi) = 0.$$

Thus the full Hartree–Fock Hessian is exactly the exchange Hessian in (4.8).

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