

# On relative bounds for interacting Fermion operators

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**Abstract.** We consider a system of interacting fermions whose Hamiltonian is unitarily transformed so that the interaction is a quartic perturbation of the Hartree–Fock effective Hamiltonian. It is shown under natural model assumptions that the interaction does not admit a relative bound with respect to the effective Hamiltonian that is uniform in the system’s size.

This bound is exemplified on the Hubbard model with nearest neighbor interaction on a discrete  $d$ -dimensional torus of length  $L$  around its Hartree–Fock ground state and derive relative bounds of the effective interaction with respect to the effective kinetic energy. It is shown that there are no relative bounds uniform in  $L$ .

## 1. Introduction and main result

All models of matter in physics and chemistry used in science and technology ultimately derive from the quantum mechanical description of interacting many-body systems. The precise description of these interacting quantum many-body systems is one of the most important tasks of mathematical and theoretical physics. The conceptual and mathematical framework was formulated almost a century ago and has not changed much since. Yet, the analysis especially of interacting systems is complex and remains challenging.

In this paper, we consider a many-fermion quantum system whose states are represented by vectors in a fermion Fock space  $\mathfrak{F} = \mathfrak{F}_f(\mathfrak{h})$ , where  $\mathfrak{h}$  is the Hilbert space of a single fermion, and a second-quantized Hamiltonian

$$\tilde{\mathbb{H}} = \mathbb{T} + \frac{g}{2}\mathbb{V} \quad (1.1)$$

acting on a suitable domain in  $\mathfrak{F}$ . Here,  $\mathbb{T}$  is a one-particle operator which is quadratic in the fields and represents the kinetic energy and external fields,  $\mathbb{V} \geq 0$  is the purely repulsive pair interaction between the fermions and quartic in the fields, and  $g > 0$  is a small coupling constant. This is the standard framework which is described with mathematical precision, e.g., in [7, 13, 14, 17, 18].

Assume the  $N$ -fermion Slater determinant  $\Phi_{\text{HF}}^{(N)} = f_1^{(\text{HF})} \wedge \cdots \wedge f_N^{(\text{HF})}$  to be a Hartree–Fock ground state. It induces a unitary particle-hole Bogoliubov transformation  $\mathbb{U}_{\text{HF}}$  on  $\mathfrak{F}$ . After Wick-ordering, the transformed Hamiltonian assumes the form

$$\mathbb{H} := \mathbb{U}_{\text{HF}}^* \tilde{\mathbb{H}} \mathbb{U}_{\text{HF}} = E_{\text{HF}}^{(N)} + \mathbb{T}_{\text{HF}} + \frac{g}{2}\mathbb{Q}, \quad (1.2)$$

where the constant  $E_{\text{HF}}^{(N)} = \langle \Omega | \mathbb{H} \Omega \rangle$  is the vacuum expectation value of the transformed Hamiltonian,  $\mathbb{T}_{\text{HF}}$  is quadratic and normal-ordered in the field operators, and  $\mathbb{Q}$  is quartic and normal-ordered in the field operators. More specifically, it turns out that  $E_{\text{HF}}^{(N)} := \langle \Phi_{\text{HF}}^{(N)} | \tilde{\mathbb{H}} \Phi_{\text{HF}}^{(N)} \rangle$  is the Hartree–Fock energy of the system and that  $\mathbb{T}_{\text{HF}} \geq 0$ , called the Hartree–Fock Hamiltonian, is the second quantization of a positive effective one-body operator. We think of (1.2) as an expansion of  $\tilde{\mathbb{H}}$  around the transformed Hartree–Fock ground state  $\Phi_{\text{HF}}^{(N)}$ , where  $\mathbb{Q}$  encodes the properties of the system beyond Hartree–Fock theory. For a review of Hartree–Fock theory we refer the reader to [2].

To develop a rigorous perturbation theory for the many-fermion system in an operator-theoretic framework, it is natural to decompose  $\mathbb{Q}$  as  $\mathbb{Q} = \mathbb{Q}_{\text{main}} + \mathbb{Q}_{\text{rem}}$ , where  $\mathbb{Q}_{\text{main}} \geq 0$  and  $\mathbb{Q}_{\text{rem}}$  is relatively bounded by  $\mathbb{T}_{\text{HF}} + \frac{g}{2} \mathbb{Q}_{\text{main}}$  with a small relative bound. The main result of this paper is that this idea fails and that, in general, there is no such decomposition. We demonstrate this statement by constructing a counterexample in several steps:

(i) In equations (3.6)–(3.9), we decompose  $\mathbb{Q}$  as

$$\mathbb{Q} = \text{Re}[\mathbb{Q}_1 + \mathbb{Q}_2 - 2\mathbb{Q}_3 + 2\mathbb{Q}_4 + 4\mathbb{Q}_5 + 4\mathbb{Q}_6 + 2\mathbb{Q}_7],$$

where  $\mathbb{Q}_{\text{main}} = \mathbb{Q}_1 + \mathbb{Q}_2$  and  $\mathbb{Q}_1 \geq 0$  and  $\mathbb{Q}_2 \geq 0$  is the particle-particle and the hole-hole repulsion, respectively.

(ii) For system of electrons (spin- $\frac{1}{2}$  fermions) on a periodic  $d$ -dimensional lattice  $\Lambda = \mathbb{Z}_L^d$  of sidelength  $L \in \mathbb{Z}^+$  with an interaction given by a repulsive pair potential  $v : \Lambda \rightarrow \mathbb{R}_0^+$  we show in Theorem 3.1 that the quadratic forms corresponding to  $\mathbb{Q}_3$ ,  $\mathbb{Q}_4$ ,  $\mathbb{Q}_5$ , and  $\mathbb{Q}_6$  are bounded relative to  $\mathbb{N} + \mathbb{Q}_{\text{main}}$ , uniformly in the thermodynamic (TD) limit, i.e., as  $L \rightarrow \infty$ . Note that  $\mathbb{N} + \mathbb{Q}_{\text{main}}$  is comparable to  $\mathbb{H}_0 = \mathbb{T}_{\text{HF}} + \mathbb{Q}_{\text{main}}$ , provided the effective one-body operator entering the Hartree–Fock Hamiltonian  $\mathbb{T}_{\text{HF}}$  is strictly positive.

(iii) Our counterexample is built on  $\mathbb{Q}_7$  which is a sum of products of four creation operators, namely, two particle and two hole creation operators. Our first main result is Theorem 3.2, in which we define a normalized trial vector  $\Phi_\varepsilon = \sqrt{1 - \varepsilon^2} \Omega + \varepsilon \|\mathbb{Q}_7 \Omega\|^{-1} \mathbb{Q}_7 \Omega$ , for  $\varepsilon \in (0, \frac{1}{2}]$ . We show that  $0 \leq \langle \Phi_\varepsilon | \mathbb{T}_{\text{HF}} \Phi_\varepsilon \rangle \leq 4\|t\|_{\text{op}}$  and  $0 \leq \langle \Phi_\varepsilon | \frac{g}{2} \mathbb{Q}_{\text{main}} \Phi_\varepsilon \rangle \leq 2g\varepsilon^2 \|v\|_{\text{op}}$  are uniformly bounded in the TD limit, provided that the one-particle kinetic energy  $t$  and the pair interaction  $v$  are bounded. In contrast,  $\langle \Phi_\varepsilon | \mathbb{Q}_7 \Phi_\varepsilon \rangle = \frac{g}{2} \|\mathbb{Q}_7 \Omega\|$ , and  $\|\mathbb{Q}_7 \Omega\|^2$  is characterized in Theorem 3.2 by (3.30), which suggests that  $\|\mathbb{Q}_7 \Omega\|^2 \sim |\Lambda| = L^d$  is an extensive quantity, at least for translation invariant systems.

(iv) In Theorem 3.3 we choose a specific model which falls into the category of models considered in (ii) and (iii) above, namely, the Hubbard model at half-filling. Following the lines of [4] for this model,  $E_{\text{HF}}^{(N)}$ ,  $\mathbb{T}_{\text{HF}}$ , and  $\mathbb{Q}$  can be explicitly computed. While any operator is relatively bounded to any other operator in case of finite-dimensional Hilbert spaces, we show here that  $\mathbb{Q}$  contains indefinite contributions  $\mathbb{Q}_{\text{rem}}$  which cannot be bounded relative to  $\mathbb{T}_{\text{HF}} + \mathbb{Q}_{\text{main}}$  with a relative bound that is *uniform in the thermodynamic (large-volume) limit*.

Note that the importance of the term  $\mathbb{Q}_7$  in the perturbative expansions for fermion systems (and also for boson systems) has been observed before in [5, 6, 9]. These go

beyond the results of the present paper in as much as unitary operators that approximately eliminate  $\mathbb{Q}_7$  have been constructed and proven to yield the next correction, e.g., in an expansion of the ground state energy in powers of the coupling constant.

In condensed matter theory, the expansion of physical quantities in powers of a small coupling constant  $g > 0$  is usually not carried out by expanding the Hamiltonian operator or its resolvent directly. One rather studies (thermal) Green's functions which encode all the physical information sought for, see, e.g., [15]. These Green's functions are then expanded in formal series in  $g$  with expansion coefficients given by sums of Feynman diagrams. In diagrammatic language, our result may be considered an attempt to sum up the contributions of all four-point ladder diagrams to the interacting four-point function. It is known that these summations often diverge, see, e.g., [16, Section 4.5], and the result of the present paper contributes to the identification of the cause for this divergence.

In the present paper the question of the validity of norm bounds for translation-invariant pair-interactions (quartic in the quantum fields) relative to a one-body operator (quadratic in the quantum fields) is investigated. This approach is adequate for weakly interacting systems and has a long history with diagrammatic expansions described above. More recently, as the theory of quantum computers developed, topologically ordered quantum lattice systems and the stability of their spectral gap has come into focus of studies. In [8] a perturbation expansion of these systems was studied, a new technique to prove relative operator bounds was developed, and the notion of quasi-adiabatic continuation was introduced which has been further developed in the past decade, see, e.g., [12] and references therein. The quasi-adiabatic continuation seems to be related to the approximate eliminations in [5, 6, 9] of terms in the Hamiltonian by conjugations with unitary operators. It would be interesting to explore the relation between these different approaches in future research projects.

## 2. $N$ -Fermion systems and Hartree–Fock approximation

**$N$ -Fermion systems.** The state of a system of  $N \in \mathbb{Z}^+ := \{1, 2, 3, \dots\}$  interacting nonrelativistic fermions at time  $t \in \mathbb{R}$  in an atom, a molecule, or a crystal is described by a wave function  $\Psi_t \in \mathfrak{F}^{(N)} \equiv \mathfrak{F}^{(N)}(\mathfrak{h})$  in, or more generally a density matrix  $\rho_t \in \mathcal{L}_+^1(\mathfrak{F}^{(N)})$  on, the  $N$ -fermion Hilbert space  $\mathfrak{F}^{(N)}(\mathfrak{h}) \subseteq \mathfrak{h}^{\otimes N}$ , which is the subspace of totally antisymmetric vectors in the  $N$ -fold tensor product of the one-particle Hilbert space  $\mathfrak{h}$ . The Hilbert space  $\mathfrak{F}^{(N)}(\mathfrak{h})$  is the closure of the span of  $N$ -fermion Slater determinants

$$f_1 \wedge \cdots \wedge f_N := (N!)^{-1/2} \sum_{\pi \in \mathcal{S}_N} (-1)^\pi f_{\pi(1)} \otimes \cdots \otimes f_{\pi(N)}.$$

Here,  $\mathcal{S}_N$  is the set of permutations of  $\{1, \dots, N\}$  and  $(-1)^\pi$  denotes their sign. If  $\{f_k\}_{k=1}^D \subseteq \mathfrak{h}$  is an orthonormal basis (ONB) then so is

$$\{f_{k(1)} \wedge \cdots \wedge f_{k(N)} \mid 1 \leq k(1) < \cdots < k(N) \leq D\} \subseteq \mathfrak{F}^{(N)}(\mathfrak{h}),$$

where  $D := \dim(\mathfrak{h}) \in \mathbb{Z}^+ \cup \{\infty\}$  is the dimension of the one-particle Hilbert space.

The dynamics of the  $N$ -fermion system is determined by the Schrödinger equation  $i\dot{\Psi}_t = H^{(N)}\Psi_t$  or  $i\dot{\rho}_t = [H^{(N)}, \rho_t]$ , respectively. Its generator is the self-adjoint Hamiltonian

$$H^{(N)} := T^{(N)} + \frac{\kappa}{2}V^{(N)}, \quad (2.1)$$

where

$$T^{(N)} := \sum_{m=1}^N T_m, \quad V^{(N)} := \sum_{m,n=1; m \neq n}^N V_{m,n},$$

$T_m$  is the one-body Hamiltonian  $t$  acting on the  $m$ th variable,  $V_{m,n}$  is the pair interaction  $v$  acting on the  $m$ th and the  $n$ th variable, and  $\kappa > 0$  is a coupling constant. That is,  $T_m = \Pi_m^* \circ (t \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1}) \circ \Pi_m$  and  $V_{m,n} = \Pi_{m,n}^* \circ (v \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1}) \circ \Pi_{m,n}$ , where  $\Pi_m$  is the natural permutation operator exchanging the factor  $f_1$  with  $f_m$ , and  $\Pi_{m,n}$  is the natural permutation operator exchanging the factors  $f_1$  with  $f_m$  and  $f_2$  with  $f_n$ , in the tensor product  $f_1 \otimes f_2 \otimes \cdots \otimes f_N$ .

The semiboundedness and self-adjointness of  $H^{(N)}$  can be ensured by the assumption that  $t : \mathfrak{s} \rightarrow \mathfrak{h}$  is a semibounded and self-adjoint linear operator defined on a dense domain  $\mathfrak{s} \subseteq \mathfrak{h}$  and that  $v : \mathfrak{s} \otimes \mathfrak{s} \rightarrow \mathfrak{h} \otimes \mathfrak{h}$  is a symmetric, nonnegative linear operator and an infinitesimal perturbation of  $t \otimes \mathbf{1} + \mathbf{1} \otimes t$ . Furthermore, we assume w.l.o.g. that  $v$  is invariant under exchanging the tensor factors in  $\mathfrak{h} \otimes \mathfrak{h}$ , i.e., that  $\text{Ex} \circ v = v \circ \text{Ex}$ , where the *exchange operator*  $\text{Ex} \in \mathcal{B}[\mathfrak{h} \otimes \mathfrak{h}]$  is defined by  $\text{Ex}(f \otimes g) = g \otimes f$ . Then  $H^{(N)}$  is semibounded and essentially self-adjoint on the subspace  $\mathfrak{F}_{\text{fin}}^{(N)}(\mathfrak{s}) \subseteq \mathfrak{F}^{(N)}(\mathfrak{h})$  of (finite) linear combinations of Slater determinants  $f_1 \wedge \cdots \wedge f_N$  with  $f_1, \dots, f_N \in \mathfrak{s}$ .

Basic quantities for the description of an  $N$ -fermion system are its ground state energy  $E_{\text{gs}}^{(N)}$  defined to the smallest expectation value of  $H^{(N)}$  evaluated on  $N$ -fermion wave functions,

$$E_{\text{gs}}^{(N)} := \inf \{ \langle \Psi^{(N)} | H^{(N)} \Psi^{(N)} \rangle \mid \Psi^{(N)} \in \mathfrak{F}^{(N)}(\mathfrak{h}) \cap \mathfrak{s}^{\otimes N}, \|\Psi^{(N)}\| = 1 \},$$

and, if existent, the corresponding minimizers  $\Psi_{\text{gs}}^{(N)} \in \mathfrak{F}^{(N)}(\mathfrak{h}) \cap \mathfrak{s}^{\otimes N}$  called ground states, which necessarily fulfill the time-independent Schrödinger equation given by

$$H^{(N)}\Psi^{(N)} = E_{\text{gs}}^{(N)}\Psi^{(N)}.$$

**Fock space, CAR, and second quantization.** It is convenient to consider  $\mathfrak{F}^{(N)}(\mathfrak{h})$  a subspace of the fermion Fock space

$$\mathfrak{F}(\mathfrak{h}) = \bigoplus_{N=0}^{\infty} \mathfrak{F}^{(N)}(\mathfrak{h}),$$

where  $\mathfrak{F}^{(0)} = \mathbb{C} \cdot \Omega$  is the one-dimensional vacuum subspace spanned by the normalized vacuum vector  $\Omega$ . We introduce the usual fermion creation operators  $\{c^*(f)\}_{f \in \mathfrak{h}} \subseteq \mathcal{B}[\mathfrak{F}]$  as follows. For a fixed orbital  $f \in \mathfrak{h}$  and  $N < D$ , these are bounded operators  $c^*(f) \in \mathcal{B}[\mathfrak{F}^{(N)}; \mathfrak{F}^{(N+1)}]$  defined by their action  $c^*(f)\Omega := f$  on the vacuum vector,

for  $N = 0$ , and  $c^*(f)[g_1 \wedge \cdots \wedge g_N] := f \wedge g_1 \wedge \cdots \wedge g_N$  on Slater determinants, for  $N \in \mathbb{Z}^+$  and  $g_1, \dots, g_N \in \mathfrak{h}$ . Extending these definitions by linearity and continuity to all of  $\mathfrak{F}$ , one obtains a family  $\{c^*(f)\}_{f \in \mathfrak{h}} \subseteq \mathcal{B}[\mathfrak{F}]$  of bounded operators on  $\mathfrak{F}$  whose norm equals  $\|c^*(f)\| = \|f\|$ . The Slater determinants can now be rewritten as  $f_1 \wedge \cdots \wedge f_N = c^*(f_1) \cdots c^*(f_N)\Omega$ , and from an ONB  $\{f_k\}_{k=1}^D \subseteq \mathfrak{h}$  of the one-particle Hilbert space we obtain ONB

$$\begin{aligned} & \{c^*(f_{k(1)}) \cdots c^*(f_{k(N)})\Omega \mid 1 \leq k(1) < \cdots < k(N) \leq D\} \subseteq \mathfrak{F}^{(N)}(\mathfrak{h}), \\ & \bigcup_{N=0}^{\infty} \{c^*(f_{k(1)}) \cdots c^*(f_{k(N)})\Omega \mid 1 \leq k(1) < \cdots < k(N) \leq D\} \subseteq \mathfrak{F}(\mathfrak{h}), \end{aligned}$$

of the  $N$ -fermion Hilbert space and the fermion Fock space, respectively.

Given an orbital  $f \in \mathfrak{h}$ , the adjoint

$$c(f) := [c^*(f)]^* \in \mathcal{B}[\mathfrak{F}]$$

of the creation operator  $c^*(f)$  is called annihilation operator. Creation and annihilation operators  $\{c^*(f), c(f)\}_{f \in \mathfrak{h}}$  form a Fock representation of the canonical anticommutation relations (CAR), i.e., for all  $f, g \in \mathfrak{h}$ ,

$$\{c^*(f), c^*(g)\} = \{c(f), c(g)\} = 0, \quad \{c(f), c^*(g)\} = \langle f \mid g \rangle \cdot \mathbf{1}_{\mathfrak{F}}, \quad c(f)\Omega = 0. \quad (2.2)$$

We introduce the number operator  $\mathbb{N}$  and the second quantizations of  $H^{(N)} = T^{(N)} + \frac{\kappa}{2}V^{(N)}$ , as defined in (2.1), and its constituents  $T^{(N)}$  and  $V^{(N)}$  by

$$\begin{aligned} \mathbb{N} &:= \bigoplus_{N=0}^{\infty} N, \quad \mathbb{T} := \bigoplus_{N=0}^{\infty} T^{(N)}, \quad \mathbb{V} := \bigoplus_{N=0}^{\infty} V^{(N)}, \\ \tilde{\mathbb{H}} &:= \bigoplus_{N=0}^{\infty} H^{(N)} = \mathbb{T} + \frac{\kappa}{2}\mathbb{V}. \end{aligned}$$

These operators are essentially self-adjoint on the subspace  $\mathfrak{F}_{\text{fin}}(\mathfrak{s}) \subseteq \mathfrak{F}(\mathfrak{h})$  of finite vectors, i.e., finite linear combinations of Slater determinants  $f_1 \wedge \cdots \wedge f_N$  with  $f_1, \dots, f_N \in \mathfrak{s}$  and varying  $N \in \mathbb{Z}_0^+$ . Using an ONB  $\{f_k\}_{k \in \mathcal{I}} \subseteq \mathfrak{s}$  of orbitals in  $\mathfrak{h}$ , where

$$\mathcal{I} := \{1, 2, \dots, D\},$$

the number operator and the second quantized operators  $\mathbb{T}$  and  $\mathbb{V}$ —and hence also  $\tilde{\mathbb{H}}$ —can be represented as  $\mathbb{N} = \sum_{k \in \mathcal{I}} c^*(f_k)c(f_k)$ ,

$$\mathbb{T} = \sum_{k, m \in \mathcal{I}} \langle f_k \mid t f_m \rangle c^*(f_k)c(f_m), \quad (2.3)$$

$$\mathbb{V} = \sum_{k, \ell, m, n \in \mathcal{I}} \langle f_k \otimes f_{\ell} \mid v(f_m \otimes f_n) \rangle c^*(f_{\ell})c^*(f_k)c(f_m)c(f_n). \quad (2.4)$$

In case of unbounded  $t$  or  $v$ , the existence of the matrix elements  $\langle f_k \mid t f_m \rangle$  and  $\langle f_k \otimes f_{\ell} \mid v(f_m \otimes f_n) \rangle$  is guaranteed by sufficient regularity of the elements of  $\mathfrak{s}$ .

**Finite dimension.** For the purpose of this paper, the unboundedness of the operators under consideration is an unnecessary complication, and we hence simply assume that the dimension

$$D = \dim(\mathfrak{h}) < \infty \quad (2.5)$$

of the one-particle Hilbert space  $\mathfrak{h}$  is finite and that  $D > N$ , where the latter requirement ensures that statements we make are not void. Consequently, the Fock space  $\mathfrak{F}(\mathfrak{h})$  is finite-dimensional, too, namely,  $\dim[\mathfrak{F}(\mathfrak{h})] = 2^D < \infty$ . Thanks to Assumption (2.5), the linear operators  $t$ ,  $v$ ,  $\mathbb{N}$ ,  $\mathbb{T}$ ,  $\mathbb{V}$ , and  $\tilde{\mathbb{H}}$  are actually all finite-dimensional self-adjoint matrices,  $\mathfrak{s} = \mathfrak{h}$  and  $\mathfrak{F}_{\text{fin}}(\mathfrak{s}) = \mathfrak{F}(\mathfrak{h})$ . The description of the theory without the assumption of finite dimension can be found, e.g., in [2]. In the end, the assertions formulated in our theorems become non-trivial in the asymptotic limit  $D > N \gg 1$ .

**Hartree–Fock approximation and Bogoliubov transformations.** The computation of the ground state energy  $E_{\text{gs}}^{(N)}$  and the corresponding ground state(s)  $\Psi_{\text{gs}}^{(N)}$  is far too complicated, due to the large dimension of the problem, even though the finiteness of  $D$  ensures their existence. The Hartree–Fock approximation described below is one of the most important methods for  $N$ -fermion systems.

The Hartree–Fock energy  $E_{\text{HF}}^{(N)}$  is defined to be the smallest expectation value of  $\tilde{\mathbb{H}}$  evaluated on  $N$ -fermion Slater determinants,

$$E_{\text{HF}}^{(N)} := \inf \{ \langle f_1 \wedge \cdots \wedge f_N \mid \tilde{\mathbb{H}} f_1 \wedge \cdots \wedge f_N \rangle \mid f_j \in \mathfrak{s}, \langle f_i \mid f_j \rangle = \delta_{i,j} \}.$$

Note that, for orthonormal  $f_1, \dots, f_N \in \mathfrak{s}$ ,

$$\langle f_1 \wedge \cdots \wedge f_N \mid \tilde{\mathbb{H}} f_1 \wedge \cdots \wedge f_N \rangle = \mathcal{E}_{\text{HF}}(\gamma) := \text{Tr}_{\mathfrak{h}}[t\gamma] + \frac{\kappa}{2} \text{Tr}_{\mathfrak{h} \otimes \mathfrak{h}}[v(\mathbf{1} - \text{Ex})(\gamma \otimes \gamma)],$$

where  $\gamma = \sum_{v=1}^N |f_v\rangle\langle f_v| = \gamma^* = \gamma^2$  is the rank- $N$  orthogonal projection onto the linear span of the orbitals  $f_1, \dots, f_N$ , and  $\text{Ex} \in \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h})$  is the exchange operator determined by  $\text{Ex}(f \otimes g) = g \otimes f$ . Therefore,

$$\begin{aligned} E_{\text{HF}}^{(N)} &= \inf \{ \mathcal{E}_{\text{HF}}(\gamma) \mid \gamma = \gamma^* = \gamma^2, \text{Tr}(\gamma) = N \} \\ &= \inf \{ \mathcal{E}_{\text{HF}}(\gamma) \mid 0 \leq \gamma \leq \mathbf{1}, \text{Tr}(\gamma) = N \}, \end{aligned} \quad (2.6)$$

where the second equality is known as Lieb’s variational principle [1, 11]. Note that

$$\{ \gamma \in \mathcal{L}^1(\mathfrak{h}) \mid 0 \leq \gamma \leq \mathbf{1}, \text{Tr}(\gamma) = 1 \} \subseteq \mathcal{L}^1(\mathfrak{h})$$

is a closed convex subset.

Thanks to  $D < \infty$ , the infimum in (2.6) is actually always a minimum attained at  $P_{\text{HF}} = \sum_{v=1}^N |f_v^{(\text{HF})}\rangle\langle f_v^{(\text{HF})}|$ , say, with orthonormal  $\{f_1^{(\text{HF})}, \dots, f_N^{(\text{HF})}\} \subseteq \mathfrak{h}$ . The minimizer(s)  $P_{\text{HF}}$ , called the Hartree–Fock ground state, fulfills a stationarity condition

$$P_{\text{HF}} = \mathbf{1}_N [h_{\text{HF}}(P_{\text{HF}})], \quad (2.7)$$

known as the Hartree–Fock equation, where  $\mathbf{1}_N$  denotes the projection onto the lowest  $N$  eigenvalues (counting multiplicities) of the Hartree–Fock effective Hamiltonian  $h_{\text{HF}}(P_{\text{HF}}) \in \mathcal{B}[\mathfrak{h}]$ , which is determined by

$$\text{Tr} [h_{\text{HF}}(\gamma)\eta] = \text{Tr}_{\mathfrak{h}}[t\eta] + \kappa \text{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} [v(\mathbf{1} - \text{Ex})(\gamma \otimes \eta)],$$

for all trace-class operators  $\eta \in \mathcal{L}^1(\mathfrak{h})$ . Assuming w.l.o.g. that the eigenvalues  $e_j^{(\text{HF})} \in \mathbb{R}$  of  $h_{\text{HF}}(P_{\text{HF}})$  are given in ascending order,  $e_1^{(\text{HF})} \leq e_2^{(\text{HF})} \leq \dots \leq e_D^{(\text{HF})}$ , we obtain an ONB  $\{f_1^{(\text{HF})}, \dots, f_D^{(\text{HF})}\} \subseteq \mathfrak{h}$  of eigenvectors of  $h_{\text{HF}}(P_{\text{HF}})$  with the first  $N$  vectors being the orbitals that enter the Hartree–Fock ground state  $P_{\text{HF}}$ . The *no unfilled shells theorem* of (unrestricted) Hartree–Fock theory [3, 4] ensures that

$$e_N^{(\text{HF})} < \mu_N := \frac{e_N^{(\text{HF})} + e_{N+1}^{(\text{HF})}}{2} < e_{N+1}^{(\text{HF})},$$

and hence that there is no paradox in equation (2.7) caused by

$$\dim \text{Ran } \mathbf{1}[h_{\text{HF}}(P_{\text{HF}}) \leq e_N^{(\text{HF})}] > N.$$

### 3. Wick-ordering and relative bounds

**Wick-ordering following a Bogoliubov transformation.** For each orbital  $f_k^{(\text{HF})}$  we abbreviate the corresponding creation and annihilation operator by  $c_k^* := c^*(f_k^{(\text{HF})})$  and  $c_k := c(f_k^{(\text{HF})})$ , respectively. Moreover, we define

$$T_{k;m} := \langle f_k^{(\text{HF})} | t f_m^{(\text{HF})} \rangle \quad \text{and} \quad V_{k,\ell;m,n} := \langle f_k^{(\text{HF})} \otimes f_\ell^{(\text{HF})} | v(f_m^{(\text{HF})} \otimes f_n^{(\text{HF})}) \rangle,$$

such that

$$\tilde{\mathbb{H}} = \sum_{k,m \in I} T_{k;m} c_k^* c_m + \frac{\kappa}{2} \sum_{k,\ell,m,n \in I} V_{k,\ell;m,n} c_\ell^* c_k^* c_m c_n.$$

Following the intuition that, for small  $v$ , the Hartree–Fock energy  $E_{\text{HF}}^{(N)}$  and the Hartree–Fock ground state  $\Phi_{\text{HF}} := f_1^{(\text{HF})} \wedge \dots \wedge f_N^{(\text{HF})} \in \mathfrak{F}^{(N)}(\mathfrak{h})$  are good approximations of the actual ground state energy  $E_{\text{gs}}^{(N)}$  and a ground state  $\Psi_{\text{gs}}$ , respectively, it is natural to introduce a unitary operator  $\mathbb{U}_{\text{HF}} \in \mathcal{U}[\mathfrak{F}(\mathfrak{h})]$  on Fock space which transforms the vacuum vector  $\Omega$  into  $\Phi_{\text{HF}} = \mathbb{U}_{\text{HF}} \Omega$ , because then the Hartree–Fock energy becomes the vacuum expectation value of  $\tilde{\mathbb{H}}$  conjugated by the unitary  $\mathbb{U}_{\text{HF}}$ ,

$$E_{\text{HF}}^{(N)} = \langle \Omega | \mathbb{U}_{\text{HF}}^* \tilde{\mathbb{H}} \mathbb{U}_{\text{HF}} \Omega \rangle,$$

as a natural offset for the energy. A unitary operator with this property is the Bogoliubov transformation  $\mathbb{U}_{\text{HF}}$  defined by  $\mathbb{U}_{\text{HF}} \Omega := \Phi_{\text{HF}}^{(N)} = c_1^* \dots c_N^* \Omega$  and

$$\mathbb{U}_{\text{HF}}^* c^*(f) \mathbb{U}_{\text{HF}} := c^*(P_{\text{HF}}^\perp f) + c(\mathfrak{j}(P_{\text{HF}} f)),$$

where

$$P_{\text{HF}} := \sum_{k=1}^N |f_k^{(\text{HF})}\rangle \langle f_k^{(\text{HF})}| \quad (3.1)$$

and  $j : \mathfrak{h} \rightarrow \mathfrak{h}$  is the antiunitary involution defined by  $j(\sum_{k=1}^D \alpha_k f_k^{(\text{HF})}) := \sum_{k=1}^D \overline{\alpha_k} f_k^{(\text{HF})}$ . Note that  $P_{\text{HF}} \circ j = j \circ P_{\text{HF}}$ . It is convenient to express this definition entirely in terms of the ONB  $\{f_k^{(\text{HF})}\}_{k=1}^D \subseteq \mathfrak{h}$  as

$$\mathbb{U}_{\text{HF}}^* c_k^* \mathbb{U}_{\text{HF}} := h_k^* + \ell_k,$$

$$h_k^* := \mathbf{1}_{\mathcal{I}(h)}(k) c_k^* \quad \text{and} \quad \ell_k := \mathbf{1}_{\mathcal{I}(\ell)}(k) c_k,$$

where  $\mathcal{I}(h) := \{k \in \mathcal{I} \mid k \geq N+1\}$  and  $\mathcal{I}(\ell) := \{k \in \mathcal{I} \mid k \leq N\}$ . Note that the operators  $\{h_k^*, h_k, \ell_k^*, \ell_k\}_{k \in \mathcal{I}}$  are again a Fock representation of the CAR, i.e., for all  $j, k \in \mathcal{I}$ ,

$$\begin{aligned} \{h_k^*, h_j^*\} &= \{h_k, h_j\} = \{\ell_k^*, \ell_j^*\} = \{\ell_k, \ell_j\} = \{h_k^*, \ell_j^*\} \\ &= \{h_k, \ell_j\} = \{h_k, \ell_j^*\} = \{h_k^*, \ell_j\} = 0, \end{aligned} \quad (3.2)$$

$$\{h_k, h_j^*\} = \delta_{k,j} \mathbf{1}_{\mathcal{I}(h)}(k), \quad \{\ell_k, \ell_j^*\} = \delta_{k,j} \mathbf{1}_{\mathcal{I}(\ell)}(k), \quad h_k \Omega = \ell_k \Omega = 0, \quad (3.3)$$

with respect to which the new number operator is

$$\mathbb{N} := \mathbb{N}_h + \mathbb{N}_\ell, \quad \text{where } \mathbb{N}_h := \sum_{k \in \mathcal{I}(h)} h_k^* h_k, \quad \mathbb{N}_\ell := \sum_{k \in \mathcal{I}(\ell)} \ell_k^* \ell_k. \quad (3.4)$$

Conjugating  $\tilde{\mathbb{H}}$  with  $\mathbb{U}_{\text{HF}}$ , we obtain the transformed Hamiltonian

$$\begin{aligned} \mathbb{H} &:= \mathbb{U}_{\text{HF}}^* \tilde{\mathbb{H}} \mathbb{U}_{\text{HF}} = \mathbb{U}_{\text{HF}}^* \mathbb{T} \mathbb{U}_{\text{HF}} + \frac{\kappa}{2} \mathbb{U}_{\text{HF}}^* \mathbb{V} \mathbb{U}_{\text{HF}} = \sum_{k,m \in \mathcal{I}} T_{k;m} (h_k^* + \ell_k) (h_m + \ell_m^*) \\ &+ \frac{\kappa}{2} \sum_{j,k,m,n \in \mathcal{I}} V_{j,k;m,n} (h_k^* + \ell_k) (h_j^* + \ell_j) (h_m + \ell_m^*) (h_n + \ell_n^*), \end{aligned}$$

and by Wick-ordering, i.e., anticommuting all creation operators  $h_k^*$  and  $\ell_k^*$  to the left and all annihilation operators  $h_k$  and  $\ell_k$  to the right, we rewrite the result in the form

$$\mathbb{H} = E_{\text{HF}}^{(N)} + \mathbb{T}_{\text{HF}} + \frac{\kappa}{2} \mathbb{Q},$$

where the first term is indeed the Hartree–Fock energy,

$$\begin{aligned} E_{\text{HF}}^{(N)} &:= \langle \Phi_{\text{HF}} \mid \mathbb{H} \Phi_{\text{HF}} \rangle \\ &= \mathcal{E}_{\text{HF}}(P_{\text{HF}}) = \text{Tr}_{\mathfrak{h}}[t P_{\text{HF}}] + \frac{\kappa}{2} \text{Tr}_{\mathfrak{h} \otimes \mathfrak{h}}[v(\mathbf{1} - \text{Ex})(P_{\text{HF}} \otimes P_{\text{HF}})], \end{aligned}$$

and serves as an energy offset. The second term  $\mathbb{T}_{\text{HF}}$  is the second quantization of the positive one-particle operator  $|h_{\text{HF}}(P_{\text{HF}}) - \mu_N|$  and, hence, itself positive. It collects all terms that are quadratic in the field operators and equals

$$\mathbb{T}_{\text{HF}} = \sum_{k \in \mathcal{I}(h)} \omega_k h_k^* h_k + \sum_{k \in \mathcal{I}(\ell)} \omega_k \ell_k^* \ell_k \geq \frac{1}{2} \omega_{\min} \mathbb{N} \geq 0, \quad (3.5)$$



where

$$\omega_k := |e_k^{(\text{HF})} - \mu_N| \quad \text{and} \quad \omega_{\min} := \min_{k \in I} \omega_k > 0,$$

and we recall that  $\mu_N = \frac{1}{2}(e_{N+1}^{(\text{HF})} + e_N^{(\text{HF})})$ . Finally, the quartic terms in the Hamiltonian are collected in  $\mathbb{Q} = \text{Re}[\mathbb{Q}_1 + \mathbb{Q}_2 - 2\mathbb{Q}_3 + 2\mathbb{Q}_4 + 4\mathbb{Q}_5 + 4\mathbb{Q}_6 + 2\mathbb{Q}_7]$ , with

$$\mathbb{Q}_1 := \sum_{j,k,m,n \in I} V_{j,k;m,n} h_k^* h_j^* h_m h_n, \quad \mathbb{Q}_2 := \sum_{j,k,m,n \in I} V_{j,k;m,n} \ell_m^* \ell_n^* \ell_k \ell_j, \quad (3.6)$$

$$\mathbb{Q}_3 := \sum_{j,k,m,n \in I} V_{j,k;m,n} h_k^* \ell_m^* \ell_j h_n, \quad \mathbb{Q}_4 := \sum_{j,k,m,n \in I} V_{j,k;m,n} h_j^* \ell_m^* \ell_k h_n, \quad (3.7)$$

$$\mathbb{Q}_5 := \sum_{j,k,m,n \in I} V_{j,k;m,n} h_k^* \ell_m^* \ell_n^* \ell_j, \quad \mathbb{Q}_6 := \sum_{j,k,m,n \in I} V_{j,k;m,n} h_j^* h_m \ell_k h_n, \quad (3.8)$$

$$\mathbb{Q}_7 := \sum_{j,k,m,n \in I} V_{j,k;m,n} h_k^* h_j^* \ell_m^* \ell_n^*. \quad (3.9)$$

**Positivity of the main interaction term  $\mathbb{Q}_{\text{main}} = \mathbb{Q}_1 + \mathbb{Q}_2$ .** We recall that the interaction potential  $V \geq 0$  is assumed to be positive. Hence, we may define  $W := V^{1/2} \geq 0$  and observe that

$$V_{j,k;m,n} = \sum_{p,q \in I} W_{j,k;p,q} W_{p,q;m,n}.$$

Introducing

$$\mathbb{A}_{p,q} := \sum_{m,n \in I} W_{p,q;m,n} h_m h_n, \quad \mathbb{B}_{p,q} := \sum_{m,n \in I} W_{m,n;p,q} \ell_n^* \ell_m,$$

we now observe that  $\mathbb{Q}_1$  and  $\mathbb{Q}_2$  are manifestly positive,

$$\mathbb{Q}_1 = \sum_{p,q} \mathbb{A}_{p,q}^* \mathbb{A}_{p,q} \geq 0, \quad \mathbb{Q}_2 = \sum_{p,q} \mathbb{B}_{p,q}^* \mathbb{B}_{p,q} \geq 0.$$

Note that both absolute, but also relative, norm bounds on  $\mathbb{Q}_1$  become large as the dimension  $D \gg N$  of the one-particle Hilbert space  $\mathfrak{h}$  grows large. The reason for this is that the number of degrees of freedom corresponding to the transformed creation operators  $h_k^*$  is  $D - N$ . Since  $\mathbb{Q}_1$  is the only term in  $\mathbb{H}$  which contains quartic terms in  $h_k^*$  and  $h_k$ , i.e., monomials in  $h_k^*$  and  $h_k$  of highest degree, it can never be relatively bounded by the other terms in the Hamiltonian with a relative bound which is uniform in  $D \rightarrow \infty$ . This fact holds true independent of the regularity properties one may assume on the interaction potential  $v$ . A similar argument applies to  $\mathbb{Q}_2$ .

It is therefore natural to integrate the terms  $\mathbb{Q}_1$  and  $\mathbb{Q}_2$  in what is considered the unperturbed Hamiltonian

$$\mathbb{H}_0 := \mathbb{T}_{\text{HF}} + \frac{\kappa}{2} \mathbb{Q}_{\text{main}} \quad \text{with} \quad \mathbb{Q}_{\text{main}} := \mathbb{Q}_1 + \mathbb{Q}_2 \geq 0,$$

and treat the remaining sum  $\mathbb{Q}_{\text{rem}} := \sum_{v=3}^7 \mathbb{Q}_v$  as a perturbation of  $\mathbb{H}_0$ ,

$$\mathbb{H} = \mathbb{H}_0 + \frac{\kappa}{2} \mathbb{Q}_{\text{rem}}.$$

In fact, one would hope that the apparent big size of  $\mathbb{Q}_1$  and  $\mathbb{Q}_2$  now turns into an advantage and helps to control the terms entering  $\mathbb{Q}_{\text{rem}}$ . For this strategy to be successful, we need to establish sufficiently strong bounds of  $\mathbb{Q}_{\text{rem}}$  relative to  $\mathbb{H}_0$ , because then the spectral properties of  $\mathbb{H}$  could be derived from those of  $\mathbb{H}_0$ , provided the coupling constant  $\kappa > 0$  is sufficiently small. The main result of this paper, however, is that this strategy fails, due to the presence of  $\mathbb{Q}_7$  in  $\mathbb{Q}_{\text{rem}}$ , see (3.9).

**Smallness of the interaction terms  $\mathbb{Q}_3, \mathbb{Q}_4, \mathbb{Q}_5$  and  $\mathbb{Q}_6$ .** To derive explicit bounds on the interaction terms  $\mathbb{Q}_v$ , we specify the model further and consider spin- $\frac{1}{2}$  particles on the periodic  $d$ -dimensional lattice  $\Lambda = \mathbb{Z}_L^d = (\mathbb{Z}/L\mathbb{Z})^d$ , such that

$$\mathfrak{h} = \ell^2(\Lambda \times \{\uparrow, \downarrow\}), \quad D = \dim(\mathfrak{h}) = 2L^d. \quad (3.10)$$

The canonical ONB in  $\mathfrak{h}$  is denoted  $\{\delta_{x,\sigma}\}_{x \in \Lambda, \sigma \in \{\uparrow, \downarrow\}} \subseteq \mathfrak{h}$ , where  $\delta_{x,\sigma}(y, \tau) := \delta_{x,y} \delta_{\sigma,\tau}$ . We introduce the corresponding creation and annihilation operators by  $c_{x,\sigma}^* := c^*(\delta_{x,\sigma})$  and  $c_{x,\sigma} = c(\delta_{x,\sigma})$ , for  $x \in \Lambda$  and  $\sigma \in \{\uparrow, \downarrow\}$ . Hence,

$$\mathfrak{F}_f(\mathfrak{h}) = \text{span} \{c_{x_1, \sigma_1}^* \cdots c_{x_N, \sigma_N}^* \Omega \mid N \in \mathbb{N}_0, x_i \in \Lambda, \sigma_i \in \{\uparrow, \downarrow\}\}. \quad (3.11)$$

The interaction  $\mathbb{V}$  in (2.4) is assumed to be of the usual form, i.e., to be induced by a nonnegative, spin-independent, pair potential  $v : \Lambda \rightarrow \mathbb{R}_0^+$ . It takes the familiar form

$$\mathbb{V} = \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} c_{x,\sigma}^* c_{y,\tau}^* c_{y,\tau} c_{x,\sigma}. \quad (3.12)$$

Defining

$$h_{x,\sigma}^* := \sum_{k \in I(h)} f_k^{(\text{HF})}(x, \sigma) c^*(f_k^{(\text{HF})}) \text{ and } \ell_{x,\sigma}^* := \sum_{k \in I(\ell)} f_k^{(\text{HF})}(x, \sigma) c^*(f_k^{(\text{HF})}), \quad (3.13)$$

we observe that

$$\begin{aligned} \{h_{x,\sigma}^*, h_{y,\tau}^*\} &= \{h_{x,\sigma}, h_{y,\tau}\} = \{\ell_{x,\sigma}^*, \ell_{y,\tau}^*\} = \{\ell_{x,\sigma}, \ell_{y,\tau}\} = \{h_{x,\sigma}^*, \ell_{y,\tau}^*\} \\ &= \{h_{x,\sigma}, \ell_{y,\tau}\} = \{h_{x,\sigma}, \ell_{y,\tau}^*\} = \{h_{x,\sigma}^*, \ell_{y,\tau}\} = 0, \end{aligned} \quad (3.14)$$

$$\{h_{x,\sigma}, h_{y,\tau}^*\} = \langle \delta_{x,\sigma} \mid P_{\text{HF}}^\perp \delta_{y,\tau} \rangle, \quad \{\ell_{x,\sigma}, \ell_{y,\tau}^*\} = \overline{\langle \delta_{x,\sigma} \mid P_{\text{HF}} \delta_{y,\tau} \rangle}, \quad (3.15)$$

$$h_{x,\sigma} \Omega = \ell_{x,\sigma} \Omega = 0, \quad (3.16)$$

for all  $x, y \in \Lambda$  and  $\sigma, \tau \in \{\uparrow, \downarrow\}$ , and

$$\mathbb{Q}_1 := \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} h_{x,\sigma}^* h_{y,\tau}^* h_{y,\tau} h_{x,\sigma}, \quad (3.17)$$

$$\mathbb{Q}_2 := \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \ell_{y,\tau}^* \ell_{x,\sigma}^* \ell_{x,\sigma} \ell_{y,\tau}, \quad (3.18)$$

$$\mathbb{Q}_3 := \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} h_{x,\sigma}^* \ell_{y,\tau}^* \ell_{y,\tau} h_{x,\sigma}, \quad (3.19)$$

$$\mathbb{Q}_4 := \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} h_{y,\tau}^* \ell_{y,\tau}^* \ell_{x,\sigma} h_{x,\sigma}, \quad (3.20)$$

$$\mathbb{Q}_5 := \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} h_{x,\sigma}^* \ell_{y,\tau}^* \ell_{x,\sigma}^* \ell_{y,\tau}, \quad (3.21)$$

$$\mathbb{Q}_6 := \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} h_{y,\tau}^* h_{y,\tau} \ell_{x,\sigma} h_{x,\sigma}, \quad (3.22)$$

$$\mathbb{Q}_7 := \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} h_{x,\sigma}^* h_{y,\tau}^* \ell_{y,\tau}^* \ell_{x,\sigma}^*. \quad (3.23)$$

Finally, we introduce the one-particle density

$$\rho_{\text{HF}}(x) := \sum_{\sigma \in \{\uparrow, \downarrow\}} \rho_{\text{HF}}(x, \sigma), \quad \rho_{\text{HF}}(x, \sigma) := \langle \delta_{x,\sigma} \mid P_{\text{HF}} \delta_{x,\sigma} \rangle \quad (3.24)$$

of the Hartree–Fock ground state at  $x \in \Lambda$  and the number operators

$$\mathbb{N}_h := \sum_{x \in \Lambda, \sigma \in \{\uparrow, \downarrow\}} h_{x,\sigma}^* h_{x,\sigma}, \quad \mathbb{N}_\ell := \sum_{x \in \Lambda, \sigma \in \{\uparrow, \downarrow\}} \ell_{x,\sigma}^* \ell_{x,\sigma}, \quad \mathbb{N} = \mathbb{N}_h + \mathbb{N}_\ell. \quad (3.25)$$

With these definitions we are in position to formulate the relative bounds on  $\mathbb{Q}_3, \mathbb{Q}_4, \mathbb{Q}_5$ , and  $\mathbb{Q}_6$  to demonstrate that these terms are under control. We remark that the bounds formulated in Theorem 3.1 below for  $\kappa = 2$ , actually hold uniformly for  $0 < \kappa \leq 2$ .

**Theorem 3.1.** *The interaction terms  $\mathbb{Q}_3, \mathbb{Q}_4, \mathbb{Q}_5$ , and  $\mathbb{Q}_6$  vanish on the vacuum sector and obey the following quadratic form bounds on the orthogonal complement of the vacuum sector:*

$$\|\mathbb{N}^{-1/2} \mathbb{Q}_3 \mathbb{N}^{-1/2}\|, \|\mathbb{N}^{-1/2} \mathbb{Q}_4 \mathbb{N}^{-1/2}\|, \|\mathbb{N}^{-1/2} \mathbb{Q}_5 \mathbb{N}^{-1/2}\| \leq 2 \|v * \rho_{\text{HF}}\|_\infty, \quad (3.26)$$

$$\|(\mathbb{N} + \mathbb{Q}_1)^{-1/2} \mathbb{Q}_6 (\mathbb{N} + \mathbb{Q}_1)^{-1/2}\| \leq \|v * \rho_{\text{HF}}\|_\infty, \quad (3.27)$$

where  $\|v * \rho_{\text{HF}}\|_\infty = \max_{x \in \Lambda} \sum_{y \in \Lambda} v(x-y) \rho_{\text{HF}}(y)$ .

*Proof.* We only need to bound the absolute value of diagonal matrix elements  $\langle \mathbb{Q}_v \rangle := \langle \Psi \mid \mathbb{Q}_v \Psi \rangle$  of normalized vectors  $\Psi \in \mathfrak{H}$ . We make multiple use of the Cauchy–Schwarz inequality  $|\langle A^* B \rangle|^2 \leq \langle A^* A \rangle \langle B^* B \rangle$ . Additionally using

$$\ell_{y,\tau}^* \ell_{y,\tau} \leq \rho_{\text{HF}}(y, \tau) \cdot \mathbf{1}_{\mathfrak{H}} \quad (3.28)$$

for the estimate of  $\mathbb{Q}_3$ , we obtain

$$\begin{aligned} |\langle \mathbb{Q}_3 \rangle| &= 2 \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \langle h_{x,\sigma}^* \ell_{y,\tau}^* \ell_{y,\tau} h_{x,\sigma} \rangle \\ &\leq 2 \sum_{x,y \in \Lambda} \sum_{\sigma \in \{\uparrow, \downarrow\}} v_{x-y} \rho_{\text{HF}}(y) \langle h_{x,\sigma}^* h_{x,\sigma} \rangle \\ &\leq 2 \|v * \rho_{\text{HF}}\|_{\infty} \langle \mathbb{N}_h \rangle \leq 2 \|v * \rho_{\text{HF}}\|_{\infty} \langle \mathbb{N} \rangle. \end{aligned}$$

By the Cauchy–Schwarz inequality and again (3.28), we have

$$\begin{aligned} |\langle \mathbb{Q}_5 \rangle| &= \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} |\langle h_{x,\sigma}^* \ell_{y,\tau}^* \ell_{x,\sigma}^* \ell_{y,\tau} \rangle| \\ &\leq \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \langle h_{x,\sigma}^* \ell_{y,\tau}^* \ell_{y,\tau} h_{x,\sigma} \rangle^{1/2} \langle \ell_{y,\tau}^* \ell_{x,\sigma} \ell_{x,\sigma}^* \ell_{y,\tau} \rangle^{1/2} \\ &\leq \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \sqrt{\rho_{\text{HF}}(x, \sigma) \rho_{\text{HF}}(y, \tau)} \langle h_{x,\sigma}^* h_{x,\sigma} \rangle^{1/2} \langle \ell_{y,\tau}^* \ell_{y,\tau} \rangle^{1/2} \\ &\leq \|v * \rho_{\text{HF}}\|_{\infty} \langle \mathbb{N}_h \rangle^{1/2} \langle \mathbb{N}_\ell \rangle^{1/2} \leq \|v * \rho_{\text{HF}}\|_{\infty} \langle \mathbb{N} \rangle. \end{aligned}$$

Next, we observe that  $\mathbb{Q}_4 = \mathbb{Q}'_4 - \mathbb{Q}''_4$ , where

$$\begin{aligned} \mathbb{Q}'_4 &:= \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \langle \delta_{x,\sigma} \mid P_{\text{HF}} \delta_{y,\tau} \rangle \langle h_{y,\tau}^* h_{x,\sigma} \rangle, \\ \mathbb{Q}''_4 &:= \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \langle h_{y,\tau}^* \ell_{x,\sigma} \ell_{y,\tau}^* h_{x,\sigma} \rangle, \end{aligned}$$

and thanks to  $|\langle \delta_{x,\sigma} \mid P_{\text{HF}} \delta_{y,\tau} \rangle|^2 \leq \rho_{\text{HF}}(x, \sigma) \rho_{\text{HF}}(y, \tau)$ , these two terms obey the estimates

$$\begin{aligned} |\langle \mathbb{Q}'_4 \rangle| &\leq \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \sqrt{\rho_{\text{HF}}(x, \sigma) \rho_{\text{HF}}(y, \tau)} \langle h_{y,\tau}^* h_{y,\tau} \rangle^{1/2} \langle h_{x,\sigma}^* h_{x,\sigma} \rangle^{1/2} \\ &\leq \|v * \rho_{\text{HF}}\|_{\infty} \langle \mathbb{N}_h \rangle, \\ |\langle \mathbb{Q}''_4 \rangle| &\leq \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \langle h_{y,\tau}^* \ell_{x,\sigma} \ell_{x,\sigma}^* h_{y,\tau} \rangle^{1/2} \langle h_{x,\sigma}^* \ell_{y,\tau} \ell_{y,\tau}^* h_{x,\sigma} \rangle^{1/2} \\ &\leq \|v * \rho_{\text{HF}}\|_{\infty} \langle \mathbb{N}_h \rangle, \end{aligned}$$

which yields  $|\langle \mathbb{Q}_4 \rangle| \leq 2 \|v * \rho_{\text{HF}}\|_{\infty} \langle \mathbb{N} \rangle$ . Finally,

$$\begin{aligned} |\langle \mathbb{Q}_6 \rangle| &\leq \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} |\langle h_{y,\tau}^* \ell_{x,\sigma} h_{y,\tau} h_{x,\sigma} \rangle| \\ &\leq \sum_{x,y \in \Lambda} \sum_{\sigma, \tau \in \{\uparrow, \downarrow\}} v_{x-y} \langle h_{y,\tau}^* \ell_{x,\sigma} \ell_{x,\sigma}^* h_{y,\tau} \rangle^{1/2} \langle h_{x,\sigma}^* h_{y,\tau}^* h_{y,\tau} h_{x,\sigma} \rangle^{1/2} \\ &\leq \|v * \rho_{\text{HF}}\|_{\infty}^{1/2} \langle \mathbb{N}_h \rangle^{1/2} \langle \mathbb{Q}_1 \rangle^{1/2}. \end{aligned}$$

■

**Main result: lower bound on  $|\langle \mathbb{Q}_7 \rangle|$ .** We come to the main result of this paper, namely a lower bound on the absolute value of  $\langle \Psi | \mathbb{Q}_7 \Psi \rangle$ , for a suitable choice of  $\Psi$ , which proves that  $\mathbb{Q}_7$  neither obeys a quadratic form bound (3.26) nor (3.27) nor any other bound that is nontrivial in the limit  $D \rightarrow \infty$ .

The absence of such a bound does not hold in general, and of course, a counterexample depends on the model. The counterexample we give is based on the Hartree–Fock ground state of the Hubbard model at half-filling because in this case the solution is explicitly known [4] – we review its construction below. We point out that this additionally illustrates that the absence of a relative bound for  $\mathbb{Q}_7$  is not caused by the long-range nature of the interaction potential – in fact, in the Hubbard model the pair interaction is  $v_{x-y} = \delta_{x,y}$ , i.e., of zero range.

Before we focus on the Hubbard model, we characterize our choice of  $\Psi$  and the main term  $\langle \Psi | \mathbb{Q}_7 \Psi \rangle$  it yields in the following theorem which, like Theorem 3.1, we formulate only for  $\kappa = 2$  – even though it actually holds true uniformly for all  $0 < \kappa \leq 2$ .

**Theorem 3.2.** *Assume that  $t \in \mathcal{B}[\mathfrak{h}]$  and  $v \in \mathcal{B}[\mathfrak{h} \otimes \mathfrak{h}]$  are bounded uniformly in  $D = \dim(\mathfrak{h})$ , and define by*

$$v_{\wedge} := \frac{1}{4}(1 - \text{Ex})v(1 - \text{Ex}) \in \mathcal{B}[\mathfrak{h} \otimes \mathfrak{h}]$$

*the restriction of  $v$  to the subspace  $\mathfrak{h} \wedge \mathfrak{h} \subseteq \mathfrak{h} \otimes \mathfrak{h}$  of antisymmetric vectors. For  $\mathbb{Q}_7$  as in (3.9) and  $\varepsilon \in (0, \frac{1}{2}]$ , define the normalized vector*

$$\Phi_{\varepsilon} := \sqrt{1 - \varepsilon^2} \Omega + \varepsilon \|\mathbb{Q}_7 \Omega\|^{-1} \mathbb{Q}_7 \Omega.$$

*Then*

$$\begin{aligned} \langle \Phi_{\varepsilon} | \mathbb{T}_{\text{HF}} \Phi_{\varepsilon} \rangle &\leq \|t\|_{\text{op}} \langle \Phi_{\varepsilon} | \mathbb{N} \Phi_{\varepsilon} \rangle \leq 4\varepsilon^2 \|t\|_{\text{op}}, \\ \langle \Phi_{\varepsilon} | \mathbb{Q}_{\text{main}} \Phi_{\varepsilon} \rangle &\leq 4\varepsilon^2 \|v\|_{\text{op}}, \\ \langle \Phi_{\varepsilon} | \mathbb{Q}_7 \Phi_{\varepsilon} \rangle &= 2\varepsilon \|\mathbb{Q}_7 \Omega\|, \end{aligned}$$

*where  $\mathbb{T}_{\text{HF}}$  is as in (3.5), and the number operator  $\mathbb{N}$  is defined in (3.4). In particular, choosing  $\varepsilon := \min\{\frac{1}{2}, (1 + \|v\|_{\text{op}})\} > 0$ , we have that*

$$\frac{\langle \Phi_{\varepsilon} | \mathbb{Q}_7 \Phi_{\varepsilon} \rangle}{\langle \Phi_{\varepsilon} | (\mathbb{T}_{\text{HF}} + \mathbb{Q}_{\text{main}} + \mathbf{1}) \Phi_{\varepsilon} \rangle} \geq \frac{\min\{\frac{1}{2}, \sqrt{1 + \|v\|_{\text{op}}}\}}{4 + \|t\|_{\text{op}}} \|\mathbb{Q}_7 \Omega\|. \quad (3.29)$$

*Furthermore,*

$$\|\mathbb{Q}_7 \Omega\|^2 = \text{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} [v_{\wedge} (P_{\text{HF}}^{\perp} \otimes P_{\text{HF}}^{\perp}) v_{\wedge} (P_{\text{HF}} \otimes P_{\text{HF}})]. \quad (3.30)$$

*Proof.* We first recall that

$$\mathbb{Q}_7 = \sum_{j,k \in I(h)} \sum_{m,n \in I(\ell)} V_{j,k;m,n} h_k^* h_j^* \ell_m^* \ell_n^*,$$

$$\begin{aligned}\mathbb{Q}_1 &= \sum_{r,s,t,u \in \mathcal{I}(h)} V_{r,s;t,u} h_s^* h_r^* h_t h_u, \\ \mathbb{Q}_2 &= \sum_{r,s,t,u \in \mathcal{I}(\ell)} V_{r,s;t,u} \ell_t^* \ell_u^* \ell_s \ell_r,\end{aligned}$$

from (3.6) and (3.9). Observe that  $\mathbb{Q}_7\Omega \perp \Omega$  because  $\mathbb{N}\Omega = 0$  and  $\mathbb{N}\mathbb{Q}_7\Omega = 4\mathbb{Q}_7\Omega$  belong to different particle number subspaces. Hence,  $\Phi_\varepsilon$  is normalized and

$$0 \leq \langle \Phi_\varepsilon | \mathbb{T}_{\text{HF}} \Phi_\varepsilon \rangle \leq \|t\|_{\text{op}} \langle \Phi_\varepsilon | \mathbb{N} \Phi_\varepsilon \rangle = 4\varepsilon^2 \|t\|_{\text{op}}. \quad (3.31)$$

Furthermore,  $\mathbb{Q}_{\text{main}} := \mathbb{Q}_1 + \mathbb{Q}_2$  preserves the particle number and  $\mathbb{Q}_{\text{main}}\Omega = 0$ . Thus

$$\langle \Phi_\varepsilon | \mathbb{Q}_{\text{main}} \Phi_\varepsilon \rangle = \varepsilon^2 \|\mathbb{Q}_7\Omega\|^{-2} (\langle \Omega | \mathbb{Q}_7^* \mathbb{Q}_1 \mathbb{Q}_7 \Omega \rangle + \langle \Omega | \mathbb{Q}_7^* \mathbb{Q}_2 \mathbb{Q}_7 \Omega \rangle). \quad (3.32)$$

Similarly, we obtain from  $\langle \Omega | \mathbb{Q}_7 \Omega \rangle = \langle \mathbb{Q}_7 \Omega | \mathbb{Q}_7^2 \Omega \rangle = 0$  that

$$\begin{aligned}\langle \Phi_\varepsilon | \text{Re}[\mathbb{Q}_7] \Phi_\varepsilon \rangle &= \varepsilon \|\mathbb{Q}_7\Omega\|^{-1} (\langle \Omega | (\mathbb{Q}_7 + \mathbb{Q}_7^*) \mathbb{Q}_7 \Omega \rangle + \langle \mathbb{Q}_7 \Omega | (\mathbb{Q}_7 + \mathbb{Q}_7^*) \Omega \rangle) \\ &= 2\varepsilon \|\mathbb{Q}_7\Omega\|^{-1} \langle \Omega | \mathbb{Q}_7^* \mathbb{Q}_7 \Omega \rangle = 2\varepsilon \|\mathbb{Q}_7\Omega\|. \quad (3.33)\end{aligned}$$

Next, we compute  $\langle \Omega | \mathbb{Q}_7^* \mathbb{Q}_7 \Omega \rangle$ ,  $\langle \Omega | \mathbb{Q}_7^* \mathbb{Q}_1 \mathbb{Q}_7 \Omega \rangle$ , and  $\langle \Omega | \mathbb{Q}_7^* \mathbb{Q}_2 \mathbb{Q}_7 \Omega \rangle$ . To this end we use (3.2) and (3.3) and obtain

$$\langle \Omega | \ell_{n'} \ell_{m'} h_{j'} h_{k'} h_k^* h_j^* \ell_m^* \ell_n^* \Omega \rangle = \langle \Omega | h_{j'} h_{k'} h_k^* h_j^* \Omega \rangle \langle \Omega | \ell_{n'} \ell_{m'} \ell_m^* \ell_n^* \Omega \rangle, \quad (3.34)$$

$$\langle \Omega | h_{j'} h_{k'} h_k^* h_j^* \Omega \rangle = (\delta_{j,j'} \delta_{k,k'} - \delta_{j,k'} \delta_{k,j'}), \quad (3.35)$$

$$\langle \Omega | \ell_{n'} \ell_{m'} \ell_m^* \ell_n^* \Omega \rangle = (\delta_{m,m'} \delta_{n,n'} - \delta_{m,n'} \delta_{n,m'}), \quad (3.36)$$

for all  $j, j', k, k' \in \mathcal{I}(h)$  and  $m, m', n, n' \in \mathcal{I}(\ell)$ . Moreover, if additionally  $t, u \in \mathcal{I}(h)$  and  $r, s \in \mathcal{I}(\ell)$  then

$$h_t h_u h_k^* h_j^* \ell_m^* \ell_n^* \Omega = (\delta_{u,k} \delta_{t,j} - \delta_{u,j} \delta_{t,k}) \ell_m^* \ell_n^* \Omega, \quad (3.37)$$

$$\ell_s \ell_r h_k^* h_j^* \ell_m^* \ell_n^* \Omega = (\delta_{r,m} \delta_{s,n} - \delta_{r,n} \delta_{s,m}) h_k^* h_j^* \Omega, \quad (3.38)$$

which imply

$$\begin{aligned}\langle \Omega | \ell_{n'} \ell_{m'} h_{j'} h_{k'} h_s^* h_r^* h_t h_u h_k^* h_j^* \ell_m^* \ell_n^* \Omega \rangle &= \langle h_r h_s h_k^* h_j^* \ell_{m'}^* \ell_{n'}^* \Omega | h_t h_u h_k^* h_j^* \ell_m^* \ell_n^* \Omega \rangle \\ &= (\delta_{s,k'} \delta_{r,j'} - \delta_{s,j'} \delta_{r,k'}) (\delta_{u,k} \delta_{t,j} - \delta_{u,j} \delta_{t,k}) \langle \ell_{m'}^* \ell_{n'}^* \Omega | \ell_m^* \ell_n^* \Omega \rangle \\ &= (\delta_{s,k'} \delta_{r,j'} - \delta_{s,j'} \delta_{r,k'}) (\delta_{u,k} \delta_{t,j} - \delta_{u,j} \delta_{t,k}) (\delta_{m,m'} \delta_{n,n'} - \delta_{m,n'} \delta_{n,m'}), \quad (3.39)\end{aligned}$$

and, similarly,

$$\begin{aligned}\langle \Omega | \ell_{n'} \ell_{m'} h_{j'} h_{k'} \ell_t^* \ell_u^* \ell_s \ell_r h_k^* h_j^* \ell_m^* \ell_n^* \Omega \rangle &= (\delta_{r,m} \delta_{s,n} - \delta_{r,n} \delta_{s,m}) (\delta_{t,m'} \delta_{u,n'} - \delta_{t,n'} \delta_{u,m'}) (\delta_{k,k'} \delta_{j,j'} - \delta_{k,j'} \delta_{j,k'}). \quad (3.40)\end{aligned}$$

Equations (3.34)–(3.40) yield

$$\begin{aligned}
\|\mathbb{Q}_7\Omega\|^2 &= \sum_{j,k,j',k' \in I(h)} \sum_{m,n,m',n' \in I(\ell)} \overline{V_{j',k';m',n'}} V_{j,k;m,n} \langle \Omega \mid \ell_{n'} \ell_{m'} h_{j'} h_{k'} h_k^* h_j^* \ell_m^* \ell_n^* \Omega \rangle \\
&= 2 \sum_{j,k \in I(h)} \sum_{m,n \in I(\ell)} V_{m,n;j,k} (V_{j,k;m,n} - V_{k,j;m,n}) \\
&= 2 \operatorname{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} [v_{\wedge} (P_{\text{HF}}^{\perp} \otimes P_{\text{HF}}^{\perp}) v_{\wedge} (P_{\text{HF}} \otimes P_{\text{HF}})],
\end{aligned}$$

where we use (3.1),  $V_{k,j;n,m} = V_{j,k;m,n}$  and  $\overline{V_{j,k;m,n}} = V_{m,n;j,k}$ , which follow from the symmetry  $\operatorname{Ex} \circ v = v \circ \operatorname{Ex}$  and the self-adjointness of  $v$ . Similarly,

$$\begin{aligned}
\langle \Omega \mid \mathbb{Q}_7^* \mathbb{Q}_1 \mathbb{Q}_7 \Omega \rangle &= 4 \sum_{j,k,r,s \in I(h)} \sum_{m,n \in I(\ell)} \overline{V_{r,s;m,n}} V_{r,s;j,k} (V_{j,k;m,n} - V_{j,k;n,m}) \\
&= 4 \operatorname{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} [v_{\wedge} (P_{\text{HF}}^{\perp} \otimes P_{\text{HF}}^{\perp}) v_{\wedge} (P_{\text{HF}}^{\perp} \otimes P_{\text{HF}}^{\perp}) v_{\wedge} (P_{\text{HF}} \otimes P_{\text{HF}})], \\
\langle \Omega \mid \mathbb{Q}_7^* \mathbb{Q}_2 \mathbb{Q}_7 \Omega \rangle &= 4 \sum_{j,k \in I(h)} \sum_{m,n,t,u \in I(\ell)} \overline{V_{j,k;t,u}} V_{m,n;t,u} (V_{j,k;m,n} - V_{j,k;n,m}) \\
&= 4 \operatorname{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} [v_{\wedge} (P_{\text{HF}} \otimes P_{\text{HF}}) v_{\wedge} (P_{\text{HF}}^{\perp} \otimes P_{\text{HF}}^{\perp}) v_{\wedge} (P_{\text{HF}} \otimes P_{\text{HF}})].
\end{aligned}$$

We abbreviate the two orthogonal projections  $P_{\text{HF}} \otimes P_{\text{HF}} =: \mathbb{P}$  and  $P_{\text{HF}}^{\perp} \otimes P_{\text{HF}}^{\perp} =: \mathbb{P}_{\perp}$ , observing that  $\mathbb{P} + \mathbb{P}_{\perp} \neq \mathbf{1}$ . With the abbreviations, we further introduce

$$\begin{aligned}
A_1 &:= \mathbb{P}_{\perp} v_{\wedge} \mathbb{P}_{\perp}, & B_1 &:= \mathbb{P}_{\perp} v_{\wedge} \mathbb{P} v_{\wedge} \mathbb{P}_{\perp} \geq 0, \\
A_2 &:= \mathbb{P} v_{\wedge} \mathbb{P}, & B_2 &:= \mathbb{P} v_{\wedge} \mathbb{P}_{\perp} v_{\wedge} \mathbb{P} \geq 0.
\end{aligned}$$

Then, for  $v = 1, 2$ , we have that

$$\langle \Omega \mid \mathbb{Q}_7^* \mathbb{Q}_v \mathbb{Q}_7 \Omega \rangle = 4 \operatorname{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} [A_v B_v] \leq 4 \|A_v\|_{\text{op}} \operatorname{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} [B_v] \leq 2 \|v\|_{\text{op}} \|\mathbb{Q}_7 \Omega\|^2,$$

and thus

$$\langle \Omega \mid \mathbb{Q}_7^* \mathbb{Q}_{\text{main}} \mathbb{Q}_7 \Omega \rangle \leq 4 \|v\|_{\text{op}} \|\mathbb{Q}_7 \Omega\|^2.$$

Equation (3.29) finally results from putting the latter estimate together with (3.32), (3.33), and (3.31).  $\blacksquare$

We are now in position to formulate our main assertion on the absence of uniform relative bounds on the example of the Hubbard model at half-filling.

**Theorem 3.3** (Absence of uniform relative bounds). *Let  $d \in \mathbb{Z}^+$ ,  $L \in 4\mathbb{Z}^+$ ,  $\Lambda = \mathbb{Z}_L^d$ ,  $\Lambda^* = \frac{2\pi}{L} \mathbb{Z}_L^d$ , and  $g > 0$ . For the Hubbard model at half-filling described in Section 4 below, it holds true that*

$$\|\mathbb{Q}_7 \Omega\|^2 \geq \frac{a}{2} |\Lambda|, \quad (3.41)$$

where

$$a := \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} \frac{\omega_{\xi}^2}{\omega_{\xi}^2 + (g/2)^2} \geq \frac{1}{4^d} \frac{d^2}{d^2 + g^2}. \quad (3.42)$$

*Proof.* We first notice that the Hubbard model falls into the category of translation invariant models specified in (3.10)–(3.25). According to (3.23), in this case  $\mathbb{Q}_7$  takes the simple form

$$\mathbb{Q}_7 = \sum_{x \in \Lambda} 2h_{x,\uparrow}^* h_{x,\downarrow}^* \ell_{x,\downarrow}^* \ell_{x,\uparrow}^*.$$

Hence

$$\begin{aligned} \|\mathbb{Q}_7 \Omega\|^2 &= 4 \sum_{x \in \Lambda} \langle \Omega \mid \ell_{x,\uparrow} \ell_{x,\downarrow} h_{x,\downarrow} h_{x,\uparrow} h_{x,\uparrow}^* h_{x,\downarrow}^* \ell_{x,\downarrow}^* \ell_{x,\uparrow}^* \Omega \rangle \\ &= 4 \sum_{x \in \Lambda} \left( \langle \delta_{x,\uparrow} \mid P_{\text{HF}}^\perp \delta_{x,\uparrow} \rangle \langle \delta_{x,\downarrow} \mid P_{\text{HF}}^\perp \delta_{x,\downarrow} \rangle - \left| \langle \delta_{x,\uparrow} \mid P_{\text{HF}}^\perp \delta_{x,\downarrow} \rangle \right|^2 \right) \\ &\quad \cdot \left( \langle \delta_{x,\uparrow} \mid P_{\text{HF}} \delta_{x,\uparrow} \rangle \langle \delta_{x,\downarrow} \mid P_{\text{HF}} \delta_{x,\downarrow} \rangle - \left| \langle \delta_{x,\uparrow} \mid P_{\text{HF}} \delta_{x,\downarrow} \rangle \right|^2 \right). \end{aligned}$$

Introducing the self-adjoint  $2 \times 2$  matrix  $M_x(\sigma, \tau) := \langle \delta_{x,\sigma} \mid P_{\text{HF}} \delta_{x,\tau} \rangle$ , we observe that  $\text{Tr}_{\mathbb{C}^2}[M_x] = \text{Tr}_{\mathbb{H}}[(\mathbf{1}_x \otimes \mathbf{1}_{\mathbb{C}^2}) P_{\text{HF}}] = 1$ , due to (A.8). Thus,  $\det[\mathbf{1} - M_x] = \det[M_x]$  and

$$\|\mathbb{Q}_7 \Omega\|^2 = 4 \sum_{x \in \Lambda} \left( \langle \delta_{x,\uparrow} \mid P_{\text{HF}} \delta_{x,\uparrow} \rangle \langle \delta_{x,\downarrow} \mid P_{\text{HF}} \delta_{x,\downarrow} \rangle - \left| \langle \delta_{x,\uparrow} \mid P_{\text{HF}} \delta_{x,\downarrow} \rangle \right|^2 \right)^2.$$

Moreover,  $\langle \delta_{x,\uparrow} \mid P_{\text{HF}} \delta_{x,\downarrow} \rangle = 0$  according to (4.5). Inserting  $\langle \delta_{x,\tau} \mid P_{\text{HF}} \delta_{x,\tau} \rangle$ , for  $\tau = \uparrow, \downarrow$ , from (4.5), we thus arrive at

$$\|\mathbb{Q}_7 \Omega\|^2 = \sum_{x \in \Lambda} (1 - 4\Delta^2) = (1 - 4\Delta^2) |\Lambda|,$$

where  $0 < \Delta < \frac{1}{2}$  is the unique solution of (4.3). It remains to show that  $\Delta < \frac{1}{2}$  uniformly in  $L \rightarrow \infty$ . To this end it is convenient to introduce

$$\mathbb{E}[X] := \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} X_\xi, \quad 0 < \varepsilon := 1 - 4\Delta^2 < 1 \quad \text{and} \quad \hat{\omega}_\xi := \frac{2\omega_\xi}{g},$$

so that (4.3) is equivalent to

$$1 = \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} \sqrt{(1 - \varepsilon + \hat{\omega}_\xi^2)^{-1}} = \mathbb{E}[\sqrt{(1 - \varepsilon + \hat{\omega}^2)^{-1}}].$$

The concavity of  $\lambda \mapsto \sqrt{\lambda}$  and Jensen's inequality imply that

$$\begin{aligned} 0 &= (\mathbb{E}[\sqrt{(1 - \varepsilon + \hat{\omega}^2)^{-1}}])^2 - 1 \leq \mathbb{E}[(1 - \varepsilon + \hat{\omega}^2)^{-1}] - 1 \\ &\leq \mathbb{E}\left[\frac{\varepsilon - \hat{\omega}^2}{1 - \varepsilon + \hat{\omega}^2}\right] \leq \frac{\varepsilon}{1 - \varepsilon} - \mathbb{E}\left[\frac{\hat{\omega}^2}{1 + \hat{\omega}^2}\right]. \end{aligned}$$

Solving this inequality for  $\varepsilon$ , we arrive at

$$\varepsilon \geq \frac{a}{1 + a} \geq \frac{a}{2}, \quad \text{with } a := \mathbb{E}\left[\frac{\hat{\omega}^2}{1 + \hat{\omega}^2}\right] \in (0, 1),$$



and, hence, at (3.41). For the derivation of (3.42) we observe that  $\cos(\frac{2\pi n_v}{L}) \geq \cos(\frac{\pi}{4}) \geq \frac{1}{2}$ , for all  $n_v + L\mathbb{Z} \in \mathbb{Z}_L$  with  $|n_v| \leq L/8$ . For each coordinate direction  $v = 1, \dots, d$ , there are at least  $L/4 \in \mathbb{Z}^+$  such  $n_v$ . Therefore,

$$\begin{aligned} a &= \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} \frac{\omega_\xi^2}{\omega_\xi^2 + (g/2)^2} \\ &\geq \frac{d^2}{d^2 + g^2} \frac{|\{\xi \in \Lambda^* : |\omega_\xi| \geq \frac{d}{2}\}|}{L^d} \geq \frac{1}{4^d} \frac{d^2}{d^2 + g^2}. \end{aligned} \quad \blacksquare$$

#### 4. Hartree–Fock theory of the Hubbard model at half-filling

**The Hubbard model at half-filling.** The Hubbard model is a simplified model for the description of interacting electrons on a discrete set  $\Lambda$  called the lattice. The single-fermion Hilbert space for this model is  $\mathfrak{h} := \ell^2(\Lambda \times \{\uparrow, \downarrow\})$ . Note that  $\mathfrak{h} \cong \mathfrak{g} \otimes \mathbb{C}^2$ , where  $\mathfrak{g} := \ell^2(\Lambda)$  is the space of complex-valued functions on  $\Lambda$ , and we frequently change between these representations without further notice.

Here we choose the lattice  $\Lambda$  to be the discrete  $d$ -dimensional torus given by  $\Lambda \equiv \Lambda_L := \mathbb{Z}_L^d$ , where  $\mathbb{Z}_L := \mathbb{Z}/L\mathbb{Z}$  and  $L \in 4\mathbb{Z}^+$  is a positive integer multiple of 4. The (Pontryagin) dual lattice is  $\Lambda^* \equiv \Lambda_L^* = \frac{2\pi}{L}\mathbb{Z}_L^d$ . The lattice  $\Lambda$  is a metric space w.r.t. the natural metric  $|x - y| := \min\{|\vec{z} - L\vec{q}|_1 : \vec{q} \in \mathbb{Z}^d\}$ , where  $\vec{z} \in \mathbb{Z}^d$  is such that  $x - y = \vec{z} + L\mathbb{Z}^d$ . Similarly,  $|\xi - \eta| := \frac{1}{L} \min\{|\vec{k} - 2\pi\vec{q}|_\infty : \vec{q} \in \mathbb{Z}^d\}$  defines a metric on  $\Lambda^*$ , where  $\vec{k} \in \mathbb{Z}^d$  such that  $\xi - \eta = \vec{k}/L + 2\pi\mathbb{Z}^d$ .

The canonical ONB with respect to coordinate space  $\Lambda$  and Fourier space  $\Lambda^*$ , respectively, are  $\{\delta_{x,\sigma}\}_{(x,\sigma) \in \Lambda \times \{\uparrow, \downarrow\}} \subseteq \mathfrak{h}$  and  $\{\varphi_{\xi,\sigma}\}_{(\xi,\sigma) \in \Lambda^* \times \{\uparrow, \downarrow\}} \subseteq \mathfrak{h}$ , where  $\delta_{x,\sigma}, \varphi_{\xi,\sigma} \in \mathfrak{h}$  are given by

$$\delta_{x,\sigma}(y, \tau) := \delta_{x,y} \delta_{\sigma,\tau} \quad \text{and} \quad \varphi_{\xi,\sigma}(y, \tau) := \frac{e^{-i\xi \cdot y}}{\sqrt{|\Lambda|}} \delta_{\sigma,\tau},$$

for all  $(y, \tau) \in \Lambda \times \{\uparrow, \downarrow\}$ , where  $\xi \cdot y = \xi_1 y_1 + \dots + \xi_d y_d$ , as usual. The fermion creation and annihilations operators corresponding to (2.2) are denoted by  $c_{x,\sigma}^* := c^*(\delta_{x,\sigma})$  and  $c_{x,\sigma} := c(\delta_{x,\sigma})$ , for  $(x, \sigma) \in \Lambda \times \{\uparrow, \downarrow\}$ , and  $\hat{c}_{\xi,\sigma}^* := c^*(\varphi_{\xi,\sigma})$  and  $\hat{c}_{\xi,\sigma} := c(\varphi_{\xi,\sigma})$ , for  $(\xi, \sigma) \in \Lambda^* \times \{\uparrow, \downarrow\}$ , respectively.

Equipped with this notation and following (1.1), we introduce the Hubbard Hamiltonian by

$$\tilde{\mathbb{H}} = \mathbb{T} + \frac{g}{2} \mathbb{V},$$

where, comparing with (3.12), the interaction  $\mathbb{V}$  is the on-site repulsion

$$v_{x-y} = \delta_{x,y}, \quad \text{i.e., } \mathbb{V} := 2 \sum_{x \in \Lambda} c_{x,\uparrow}^* c_{x,\downarrow}^* c_{x,\downarrow} c_{x,\uparrow},$$

and the kinetic energy

$$\mathbb{T} := \sum_{x,y \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} t_{x-y} c_{x,\sigma}^* c_{y,\sigma} = \sum_{\xi \in \Lambda^*} \sum_{\sigma=\uparrow,\downarrow} \omega_\xi \hat{c}_{\xi,\sigma}^* \hat{c}_{\xi,\sigma}$$

is the second quantization of the (traceless) discrete Laplacian. That is,  $T = (t_{x-y})_{x,y \in \Lambda}$  is the nearest-neighbour hopping matrix,  $T = T^* \in \mathbb{C}^{\Lambda \times \Lambda}$ , and  $\omega = \hat{t}$  is its Fourier transform,

$$t_z := -\mathbf{1}(|z| = 1) \quad \text{and} \quad \omega_\xi := \sum_{z \in \Lambda} e^{-i\xi \cdot z} t_z = -\sum_{v=1}^d \cos(\xi_v).$$

Before describing the Hartree–Fock theory on the example of the Hubbard model, we discuss the special spectral properties of the hopping matrix  $T$  that allow us to determine the Hartree–Fock minimizers explicitly.

The hopping matrix  $T$  is *bipartite*, i.e., the lattice  $\Lambda = A \dot{\cup} B$  is the union of two disjoint subsets  $A, B \subseteq \Lambda$  such that  $T_{x,y} = 0$  whenever either  $x, y \in A$  or  $x, y \in B$ . Introducing a unitary (gauge) transformation  $G \in \mathcal{U}[\ell^2(\Lambda)]$  on the functions on  $\Lambda$  by

$$[G\psi](x) := (-1)^x \psi(x), \quad \text{where } (-1)^x := \mathbf{1}_A(x) - \mathbf{1}_B(x),$$

it is easy to check that  $G$  is an involution and that  $T$  transforms under conjugation with  $G$  as

$$GTG = -T.$$

This implies that the eigenvalues of  $T$  come in pairs of opposite sign and that the projections onto its negative and positive eigenvalues, respectively, have the same dimension.

In the present case  $\Lambda \equiv \Lambda_L := \mathbb{Z}_L^d$ , the subsets  $A$  and  $B$  are the even and odd sites, respectively, forming a chessboard structure on  $\Lambda$ . More specifically,  $x = (x_1, \dots, x_d) \in \Lambda$  belongs to  $A$  or  $B$  if  $x_1 + \dots + x_d$  is even or odd, respectively, and  $G$  acts on wave functions at  $x$  by multiplication with

$$(-1)^x = (-1)^{x_1} \dots (-1)^{x_d}.$$

In Fourier representation,  $G$  acts as a translation of momenta by

$$\pi := (\pi, \dots, \pi) = -\pi \in \Lambda^*,$$

i.e.,  $G\varphi_{\xi,\sigma} = \varphi_{\xi+\pi,\sigma}$ , which is consistent with  $\omega_{\xi-\pi} = -\omega_\xi$  when conjugating  $T$  with  $G$ . Note that the translation  $\xi \mapsto \xi + \pi$  is a bijection  $\Lambda^* \rightarrow \Lambda^*$  without any fixed point. We collect the momenta corresponding to strictly positive eigenvalues and to strictly negative eigenvalues, respectively, in

$$\tilde{\Lambda}_+^* := \{\xi \in \Lambda \mid \omega_\xi > 0\} \quad \text{and} \quad \tilde{\Lambda}_-^* := \{\xi \in \Lambda \mid \omega_\xi < 0\},$$

and observe that, due to  $\omega_{\xi-\pi} = -\omega_\xi$ , the map  $\xi \mapsto \xi + \pi$  is an involution  $\Lambda_+^* \rightarrow \Lambda_-^*$ . Since the bijection  $\Lambda^* \ni \xi \mapsto \xi + \pi \in \Lambda^*$  leaves  $\tilde{\Lambda}_0^* := \{\xi \in \Lambda \mid \omega_\xi = 0\} = \tilde{\Lambda}_0^* + \pi$  invariant, but has no fixed point, we can find a disjoint partition  $\tilde{\Lambda}_0^* = \tilde{\Lambda}_{0,+}^* \dot{\cup} \tilde{\Lambda}_{0,-}^*$  such that  $\xi \mapsto \xi + \pi$  is an involution  $\tilde{\Lambda}_{0,-}^* \rightarrow \tilde{\Lambda}_{0,+}^*$ . It follows that

$$\Lambda_+^* = \tilde{\Lambda}_+^* \cup \tilde{\Lambda}_{0,+}^* \quad \text{and} \quad \Lambda_-^* = \tilde{\Lambda}_-^* \cup \tilde{\Lambda}_{0,-}^* \quad (4.1)$$

form a disjoint partition of  $\Lambda = \Lambda_+^* \dot{\cup} \Lambda_-^*$  such that  $\xi \mapsto \xi + \pi$  is a bijection from  $\Lambda_+^*$  to  $\Lambda_-^*$  (and therefore also from  $\Lambda_-^*$  to  $\Lambda_+^*$ ).

We are now in position to formulate the Hartree–Fock theory for the Hubbard model [4]. According to Lieb’s variational principle [1, 10], the Hartree–Fock energy of the Hubbard model for  $N$  electrons is given by

$$E_{\text{HF}}(N) := \inf \{ \mathcal{E}_{\text{HF}}(\gamma) \mid \gamma \in \mathcal{L}^1(\mathfrak{h}), 0 \leq \gamma \leq \mathbf{1}, \text{Tr}(\gamma) = N \}, \quad (4.2)$$

where the Hartree–Fock functional  $\mathcal{E}_{\text{HF}}$  is defined as

$$\begin{aligned} \mathcal{E}_{\text{HF}}(\gamma) &:= \text{Tr}_{\mathfrak{h}} [(T \otimes \mathbf{1})\gamma] + g \sum_{x \in \Lambda} \sum_{\sigma, \tau = \uparrow, \downarrow} \{ \langle \delta_{x, \sigma} \mid \gamma \delta_{x, \sigma} \rangle \langle \delta_{x, \tau} \mid \gamma \delta_{x, \tau} \rangle - | \langle \delta_{x, \sigma} \mid \gamma \delta_{x, \tau} \rangle |^2 \} \\ &= \text{Tr}_{\mathfrak{h}} [(T \otimes \mathbf{1})\gamma] + g \sum_{x \in \Lambda} \{ [\text{Tr}_{\mathbb{C}^2}(\gamma_x)]^2 - \text{Tr}_{\mathbb{C}^2}(\gamma_x^2) \}, \end{aligned}$$

and  $\gamma_x \in \mathbb{C}^{2 \times 2}$  is given as  $\gamma_x(\sigma, \tau) := \langle \delta_{x, \sigma} \mid \gamma \delta_{x, \tau} \rangle$ .

We recall that any self-adjoint matrix  $A = A^* \in \mathbb{C}^{2 \times 2}$  can be written as

$$A = \frac{1}{2}(\rho(A)\mathbf{1}_{\mathbb{C}^2} + \vec{v}(A) \cdot \vec{\sigma}),$$

where  $\rho(A) := \text{Tr}_{\mathbb{C}^2}(A)$ ,  $\vec{v}(A) := \text{Tr}_{\mathbb{C}^2}(\vec{\sigma}A)$ , and  $\vec{\sigma} = (\sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)})$  are the (traceless) Pauli matrices  $\sigma^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ,  $\sigma^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ , and  $\sigma^{(3)} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ . Since  $\text{Tr}(A^2) = \frac{1}{2}\rho(A) + \frac{1}{2}|\vec{v}(A)|^2$ , it follows that

$$[\text{Tr}_{\mathbb{C}^2}(\gamma_x)]^2 - \text{Tr}_{\mathbb{C}^2}(\gamma_x^2) = \frac{1}{2}\rho_x^2 - \frac{1}{2}|\vec{v}_x|^2,$$

where

$$\rho_x := \rho(\gamma_x) = \text{Tr}_{\mathfrak{h}}[(\mathbf{1}_x \otimes \mathbf{1})\gamma] \quad \text{and} \quad \vec{v}_x := \vec{v}(\gamma_x) = \text{Tr}_{\mathfrak{h}}[(\mathbf{1}_x \otimes \vec{\sigma})\gamma].$$

Moreover, with these definitions,  $0 \leq \gamma_x \leq \mathbf{1}_{\mathbb{C}^2}$  is equivalent to  $0 \leq |\vec{v}_x| \leq \rho_x \leq 2$  and we obtain

$$\mathcal{E}_{\text{HF}}(\gamma) = \text{Tr}_{\mathfrak{h}}[(T \otimes \mathbf{1})\gamma] + \frac{g}{2} \sum_{x \in \Lambda} \{ \rho_x^2 - |\vec{v}_x|^2 \}.$$

Next, we characterize the Hartree–Fock energy  $E_{\text{HF}}(|\Lambda|)$  and Hartree–Fock ground states. The latter are 1-RDM  $\gamma$  of particle number  $\text{Tr}(\gamma) = |\Lambda|$ , for which the Hartree–Fock energy is attained,  $\mathcal{E}_{\text{HF}}(\gamma) = E_{\text{HF}}(|\Lambda|)$ , see [4].

**Theorem 4.1.** *Let  $g > 0$ .*

(i) *The Hartree–Fock energy per unit volume is given by*

$$\frac{E_{\text{HF}}(|\Lambda|)}{|\Lambda|} = \frac{g}{2} + g\Delta^2 - \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} \sqrt{\omega_{\xi}^2 + g^2\Delta^2},$$

where  $\Delta \in (0, \frac{1}{2})$  is the unique solution of

$$2 = \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} g(\omega_{\xi}^2 + g^2\Delta^2)^{-1/2}. \quad (4.3)$$

- (ii) A reduced one-particle density matrix  $\gamma \in \mathcal{L}^1(\mathfrak{h})$ ,  $0 \leq \gamma \leq \mathbf{1}$ , of particle number  $\text{Tr}(\gamma) = |\Lambda|$  is a Hartree–Fock ground state if, and only if there exists a vector  $\vec{e} \in \mathbb{R}^3$  of unit length  $|\vec{e}| = 1$  such that

$$\gamma = \mathbf{1}[T \otimes \mathbf{1} - g\Delta G \otimes (\vec{e} \cdot \vec{\sigma}) \leq 0]. \quad (4.4)$$

We observe that, for any  $\vec{e} \in \mathbb{R}^3$  of unit length there is a unitary rotation  $R_{\vec{e}} \in \mathcal{U}(\mathbb{C}^2)$  in spin space such that  $R_{\vec{e}}(\vec{e} \cdot \vec{\sigma})R_{\vec{e}}^* = -\vec{e}_3 \cdot \vec{\sigma} = -\sigma^{(3)}$ . Hence, for  $r > 0$ ,

$$H_r := T \otimes \mathbf{1} + rG \otimes \sigma^{(3)} = (\mathbf{1} \otimes R_{\vec{e}})[T \otimes \mathbf{1} - rG \otimes (\vec{e} \cdot \vec{\sigma})](\mathbf{1} \otimes R_{\vec{e}})^*,$$

and we may henceforth assume w.l.o.g. that  $\vec{e} = -\vec{e}_3 = (0, 0, -1)^t$ . We observe that  $H_r$  leaves the two-dimensional subspaces  $\mathfrak{h}(\xi, \sigma) := \mathbb{C}\varphi_{\xi, \sigma} \oplus \mathbb{C}\varphi_{\xi + \pi, \sigma}$  invariant, for each  $(\xi, \sigma) \in \Lambda_+^* \times \{\uparrow, \downarrow\}$  and all  $r > 0$ . More specifically,

$$H_r = \bigoplus_{(\xi, \sigma) \in \Lambda_+^* \times \{\uparrow, \downarrow\}} H_r(\xi, \sigma), \quad \text{with } H_r(\xi, \sigma) = \begin{pmatrix} \omega_\xi & \sigma r \\ \sigma r & -\omega_\xi \end{pmatrix}$$

w.r.t. the ONB  $\{\varphi_{\xi, \sigma}, \varphi_{\xi + \pi, \sigma}\} \subseteq \mathfrak{h}(\xi, \sigma)$ , where here and henceforth we identify  $\uparrow \equiv +1$  and  $\downarrow \equiv -1$ . Fixing  $(\xi, \sigma) \in \Lambda_+^* \times \{\uparrow, \downarrow\}$ , an ONB  $\{\psi_{\xi, \sigma, +}^{(r)}, \psi_{\xi, \sigma, -}^{(r)}\} \subseteq \mathfrak{h}(\xi, \sigma)$  of eigenvectors of  $H_r(\xi, \sigma)$  with corresponding eigenvalues  $\pm \lambda_\xi^{(r)}$  is given by

$$\begin{aligned} \psi_{\xi, \sigma, \kappa}^{(r)} &= \frac{\sigma}{\sqrt{2}} a_{\xi, \kappa}^{(r)} \varphi_{\xi, \sigma} + \frac{\kappa}{\sqrt{2}} a_{\xi, -\kappa}^{(r)} \varphi_{\xi + \pi, \sigma}, \\ a_{\xi, \kappa}^{(r)} &:= \sqrt{1 + \kappa \frac{\omega_\xi}{\sqrt{\omega_\xi^2 + r^2}}}, \\ \lambda_\xi^{(r)} &= \sqrt{\omega_\xi^2 + r^2}, \end{aligned}$$

for  $(\xi, \sigma, \kappa) \in \Lambda_+^* \times \{\uparrow, \downarrow\} \times \{\pm 1\}$  with  $\{\pm 1\} := \{-1, 1\}$ . We frequently omit to display the dependence on  $r > 0$  and simply write  $\psi_{\xi, \sigma, \kappa} \equiv \psi_{\xi, \sigma, \kappa}^{(r)}$ ,  $a_{\xi, \kappa} \equiv a_{\xi, \kappa}^{(r)}$ , and  $\lambda_{\xi, \kappa} \equiv \lambda_{\xi, \kappa}^{(r)}$ .

The projection onto the Hartree–Fock ground state corresponding to  $\vec{e} = (0, 0, -1)^t$  is hence given as  $P_{\text{HF}} = \gamma^{(g\Delta)}$  where  $\gamma^{(r)} := \mathbf{1}[H_r \leq 0]$ , for  $r > 0$ . Note that  $\gamma^{(r)} = \mathbf{1}[H_r < 0]$ , because all eigenvalues of  $H_r$  are nonvanishing. Moreover, we have the explicit representation

$$\gamma^{(r)} = \sum_{(\xi, \sigma) \in \Lambda_+^* \times \{\uparrow, \downarrow\}} |\psi_{\xi, \sigma, -}\rangle \langle \psi_{\xi, \sigma, -}|.$$

Since

$$\langle \delta_{x, \tau} | \psi_{\xi, \sigma, -} \rangle = \frac{\delta_{\sigma, \tau}}{\sqrt{2}} \frac{e^{-i\xi \cdot x}}{\sqrt{|\Lambda^*|}} [\sigma a_{\xi, -} - (-1)^x a_{\xi, +}],$$

a simple computation yields

$$\gamma_x^{(r)}(\sigma, \tau) := \langle \delta_{x, \sigma} | \gamma^{(r)} | \delta_{x, \tau} \rangle = \frac{\delta_{\sigma, \tau}}{2} \left[ 1 - \frac{\tau(-1)^x r}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} (\omega_\xi^2 + r^2)^{-1/2} \right].$$

Especially for  $r = g\Delta$ , the self-consistent equation (4.3) implies that

$$\langle \delta_{x,\sigma} | P_{\text{HF}} \delta_{x,\tau} \rangle = \delta_{\sigma,\tau} \left( \frac{1}{2} - \tau(-1)^x \Delta \right). \quad (4.5)$$

### A. Proof of Theorem 4.1

We follow [4]. Let

$$\mathcal{F}_L(\eta) := g\eta - \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} \sqrt{\omega_\xi^2 + g^2 \eta}. \quad (A.1)$$

We first show that

$$E_{\text{HF}}(|\Lambda|) |\Lambda|^{-1} \geq \frac{g}{2} + \min_{0 \leq \eta \leq 4} \{ \mathcal{F}_L(\eta) \}.$$

To this end we observe that

$$|\Lambda|^2 = \left( \sum_{x \in \Lambda} \rho_x \right)^2 \leq |\Lambda| \sum_{x \in \Lambda} \rho_x^2,$$

by the Cauchy–Schwarz inequality. Hence,

$$\mathcal{E}_{\text{HF}}(\gamma) - \frac{g}{2} |\Lambda| \geq \mathcal{E}'_{\text{HF}}(\gamma) := \text{Tr}_{\mathfrak{h}} [(T \otimes \mathbf{1})\gamma] - \frac{g}{2} \sum_{x \in \Lambda} |\vec{w}_x|^2. \quad (A.2)$$

Note that  $\mathcal{E}_{\text{HF}}(\gamma) - \frac{g}{2} |\Lambda| = \mathcal{E}'_{\text{HF}}(\gamma)$  if, and only if,  $\rho_x = 1$ , for all  $x \in \Lambda$ .

A trivial, but important, observation is that  $\vec{v}_x \geq 2\vec{v}_x \cdot \vec{w}_x - \vec{w}_x^2 \geq 0$ , for any  $\vec{w}_x \in \mathbb{R}^3$ , with strict inequality unless  $\vec{w}_x = \vec{v}_x$ . Taking  $|\vec{v}_x| \leq 2$  into account, this leads to

$$|\vec{v}_x|^2 = \max_{|\vec{w}_x| \leq 2} \{ 2\vec{v}_x \cdot \vec{w}_x - |\vec{w}_x|^2 \}$$

and in turn to

$$\begin{aligned} \mathcal{E}'_{\text{HF}}(\gamma) &\geq \min_{\underline{w}} \left\{ \text{Tr}_{\mathfrak{h}} [(T \otimes \mathbf{1})\gamma] - \sum_{x \in \Lambda} g \vec{w}_x \cdot \vec{v}_x + \frac{g}{2} \sum_{x \in \Lambda} |\vec{w}_x|^2 \right\} \\ &= \min_{\underline{w}} \left\{ \text{Tr}_{\mathfrak{h}} \left[ \left( T \otimes \mathbf{1} - \sum_{x \in \Lambda} g E_{x,x} \otimes \vec{w}_x \cdot \vec{\sigma} \right) \gamma \right] + \frac{g}{2} \sum_{x \in \Lambda} |\vec{w}_x|^2 \right\}, \end{aligned}$$

where  $E_{x,y} \in \mathcal{B}[\ell^2(\Lambda)]$  is the matrix unit corresponding to  $(x, y) \in \Lambda^2$ , and  $\min_{\underline{w}}$  denotes the minimum over  $\underline{w} = (\vec{w}_x)_{x \in \Lambda} \in \overline{B_{\mathbb{R}^3}(0, 2)}^{|\Lambda|}$ . Inserting this into (4.2), we obtain the lower bound

$$\begin{aligned} E_{\text{HF}}(|\Lambda|) - \frac{g}{2} |\Lambda| &\geq \min_{\underline{w}} \left\{ \inf_{0 \leq \gamma \leq 1} \left( \text{Tr}_{\mathfrak{h}} \left[ \left( T \otimes \mathbf{1} - \sum_{x \in \Lambda} g E_{x,x} \otimes \vec{w}_x \cdot \vec{\sigma} \right) \gamma \right] + \frac{g}{2} \sum_{x \in \Lambda} |\vec{w}_x|^2 \right) \right\} \\ &= \min_{\underline{w}} \left\{ \text{Tr}_{\mathfrak{h}} \left[ \left( T \otimes \mathbf{1} - \sum_{x \in \Lambda} g E_{x,x} \otimes \vec{w}_x \cdot \vec{\sigma} \right)_- \right] + \frac{g}{2} \sum_{x \in \Lambda} |\vec{w}_x|^2 \right\}, \end{aligned}$$

where  $(\lambda)_- := \min\{\lambda, 0\} = -\frac{1}{2}|\lambda| + \frac{1}{2}\lambda = -\frac{1}{2}\sqrt{\lambda^2} + \frac{1}{2}\lambda$  denotes the negative part of a real number  $\lambda$ . Since both  $T \in \mathcal{B}[\ell^2(\Lambda)]$  and  $\sigma^{(v)} \in \mathbb{C}^{2 \times 2}$  are traceless, so is  $T \otimes \mathbf{1} -$

$\sum_{x \in \Lambda} g E_{x,x} \otimes \vec{w}_x \cdot \vec{\sigma} \in \mathcal{B}[\mathfrak{h}]$  and hence

$$E_{\text{HF}}(|\Lambda|) - \frac{g}{2} |\Lambda| \geq \frac{1}{2} \min_{\underline{w}} \left\{ \text{Tr}_{\mathfrak{h}} \left( -\sqrt{A(\underline{w})} \right) + g \sum_{x \in \Lambda} |\vec{w}_x|^2 \right\}, \quad (\text{A.3})$$

where

$$\begin{aligned} A(\underline{w}) &:= T^2 \otimes \mathbf{1} + \sum_{x \in \Lambda} g^2 |\vec{w}_x|^2 E_{x,x} \otimes \mathbf{1} - g \left\{ T \otimes \mathbf{1}, \sum_{x \in \Lambda} E_{x,x} \otimes \vec{w}_x \cdot \vec{\sigma} \right\} \\ &= T^2 \otimes \mathbf{1} + \sum_{x \in \Lambda} g^2 |\vec{w}_x|^2 E_{x,x} \otimes \mathbf{1} - \sum_{x,y \in \Lambda} g t_{x-y} E_{x,y} \otimes (\vec{w}_x + \vec{w}_y) \cdot \vec{\sigma}, \end{aligned}$$

with  $\{A, B\} := AB + BA$  denoting the anticommutator of two operators  $A$  and  $B$ . Since  $GE_{y,y}G = E_{y,y}$  and  $GTG = -T$ , we have that

$$GA(\underline{w})G = A(-\underline{w}). \quad (\text{A.4})$$

Furthermore, the strict convexity of  $\mathbb{R}_0^+ \ni \lambda \mapsto -\sqrt{\lambda} \in \mathbb{R}$  implies the strict convexity of

$$A \mapsto \text{Tr}[-\sqrt{A}], \quad (\text{A.5})$$

as a map on self-adjoint positive operators. Equations (A.4) and (A.5) imply that

$$\begin{aligned} &\text{Tr}_{\mathfrak{h}}[-\sqrt{A(\underline{w})}] \\ &= \frac{1}{2} \text{Tr}_{\mathfrak{h}}[-\sqrt{A(\underline{w})}] + \frac{1}{2} \text{Tr}_{\mathfrak{h}}[-\sqrt{A(-\underline{w})}] \geq \text{Tr}_{\mathfrak{h}} \left[ -\sqrt{\frac{1}{2}A(\underline{w}) + \frac{1}{2}A(-\underline{w})} \right] \\ &= -\text{Tr}_{\mathfrak{h}} \left[ \left( T^2 + \sum_{x \in \Lambda} g^2 |\vec{w}_x|^2 E_{x,x} \right)^{1/2} \otimes \mathbf{1} \right] \\ &= -2 \text{Tr}_{\mathfrak{g}} \left[ \left( T^2 + \sum_{x \in \Lambda} g^2 |\vec{w}_x|^2 E_{x,x} \right)^{1/2} \right], \end{aligned} \quad (\text{A.6})$$

with strict inequality unless  $t_{x-y}(\vec{w}_x + \vec{w}_y) = 0$ , for all  $x, y \in \Lambda$ . Here we use that  $\mathfrak{h} = \mathfrak{g} \otimes \mathbb{C}^2$ , where  $\mathfrak{g} := \ell^2(\Lambda)$  denotes the space of complex-valued functions on  $\Lambda$ .

Next, we introduce by  $\tau^z \in \mathcal{U}[\mathfrak{g}]$  the translation of wave functions by  $z \in \Lambda$ . That is,  $[\tau^z \psi](x) := \psi(x - z)$ , for all  $x \in \Lambda$ , and  $(\tau^z)^* = \tau^{-z}$ . Then  $\tau^z T \tau^{-z} = T$  and  $\tau^z E_{x,y} \tau^{-z} = E_{x+z, y+z}$ . Again the strict convexity (A.5) implies that

$$\begin{aligned} &-\text{Tr}_{\mathfrak{g}} \left[ \left( T^2 + \sum_{x \in \Lambda} g^2 |\vec{w}_x|^2 E_{x,x} \right)^{1/2} \right] \\ &= -\frac{1}{|\Lambda|} \sum_{z \in \Lambda} \text{Tr}_{\mathfrak{g}} \left[ \tau^z \left( T^2 + \sum_{x \in \Lambda} g^2 |\vec{w}_x|^2 E_{x,x} \right)^{1/2} \tau^{-z} \right] \\ &\geq -\text{Tr}_{\mathfrak{g}} \left[ \left( T^2 + \frac{1}{|\Lambda|} \sum_{x,z \in \Lambda} g^2 |\vec{w}_x|^2 E_{x-z, x-z} \right)^{1/2} \right] \\ &= -\text{Tr}_{\mathfrak{g}} \left[ \sqrt{T^2 + g^2 \langle \vec{w}^2 \rangle} \right] = -\sum_{\xi \in \Lambda^*} \sqrt{\omega_{\xi}^2 + g^2 \langle \vec{w}^2 \rangle}, \end{aligned}$$

where  $\langle \vec{w}^2 \rangle := \frac{1}{|\Lambda|} \sum_{x \in \Lambda} |\vec{w}_x|^2 \in [0, 4]$ , with strict inequality unless  $|\vec{w}_x|$  is independent of  $x \in \Lambda$ . Inserting this and (A.6) into (A.3), we obtain

$$E_{\text{HF}}(|\Lambda|)|\Lambda|^{-1} \geq \frac{g}{2} + \min_{0 \leq \eta \leq 4} \{ \mathcal{F}_L(\eta) \}$$

with  $\mathcal{F}_L : \mathbb{R}_0^+ \rightarrow \mathbb{R}$  as defined in (A.1),

$$\mathcal{F}_L(\eta) := g\eta - \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} (\omega_\xi^2 + g^2\eta)^{1/2}.$$

Note that  $\mathcal{F}_L \in C^\infty(\mathbb{R}^+; \mathbb{R})$  with

$$\mathcal{F}'_L(\eta) = g - \frac{g^2}{2} \frac{1}{|\Lambda^*|} \sum_{\xi \in \Lambda^*} (\omega_\xi^2 + g^2\eta)^{-1/2}$$

and  $\mathcal{F}''_L(\eta) > 0$ , for  $\eta > 0$ . Since  $L \in 4\mathbb{Z}^+$ , we have that

$$\frac{1}{2}\pi = \left( \frac{1}{2}\pi, \dots, \frac{1}{2}\pi \right) \in \Lambda^*$$

with  $\omega_{\frac{1}{2}\pi} = \sum_{v=1}^d \cos(\pi/2) = 0$ . This implies that  $\lim_{\eta \rightarrow 0} \mathcal{F}'_L(\eta) = -\infty$ . Furthermore,  $\mathcal{F}'_L(\eta) > g(1 - \frac{1}{2\sqrt{\eta}}) \geq 0$ , for any  $\eta \geq \frac{1}{4}$ . It follows that the minimum of  $\mathcal{F}_L$  is attained for the unique solution  $0 < \Delta^2 < \frac{1}{4}$  of (4.3) and that

$$\frac{E_{\text{HF}}(|\Lambda|)}{|\Lambda|} \geq \frac{g}{2} + \mathcal{F}_L(\Delta^2).$$

Next we show that this lower bound is attained precisely by the projections defined in (4.4). To this end we introduce

$$H(\vec{a}) := T \otimes \mathbf{1} + G \otimes (\vec{a} \cdot \vec{\sigma}) \quad \text{and} \quad \gamma(\vec{a}) := \mathbf{1}[H(\vec{a}) \leq 0],$$

for any  $\vec{a} \in \mathbb{R}^3 \setminus \{0\}$ . Note that zero is not an eigenvalue of  $H(\vec{a})$  because

$$H(\vec{a})^2 = (T^2 + |\vec{a}|^2) \otimes \mathbf{1} \geq |\vec{a}|^2 > 0.$$

Therefore,  $\gamma(\vec{a}) = \mathbf{1}[H(\vec{a}) < 0]$  is the projection onto the negative eigenvalues of  $H(\vec{a})$  independent of its functional form at zero, and

$$\gamma(\vec{a}) = \frac{1}{2} \mathbf{1} - F[H(\vec{a})] \tag{A.7}$$

where  $F \in C^\infty(\mathbb{R}; \mathbb{R})$  is an odd function  $F[-\lambda] = -F[\lambda]$  with  $F \equiv 1$  on  $(\frac{1}{2}|\vec{a}|, \infty)$ .

If  $\vec{b} \in \mathbb{R}^3$  is a unit vector perpendicular to  $\vec{a}$  then  $\vec{b} \cdot \vec{\sigma} \in \mathcal{U}[\mathbb{C}^2]$  is a unitary involution and  $(\vec{b} \cdot \vec{\sigma})(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = -\vec{a} \cdot \vec{\sigma}$ . Since furthermore  $GTG = -T$ , this implies that

$$U_{\vec{b}} H(\vec{a}) U_{\vec{b}} = -H(\vec{a}), \quad U_{\vec{b}} := U_{\vec{b}}^* := G \otimes (\vec{b} \cdot \vec{\sigma}) \in \mathcal{U}[\mathfrak{h}],$$

and further

$$\begin{aligned} \text{Tr}_{\mathfrak{h}} \{ (\mathbf{1}_x \otimes \mathbf{1}) F[H(\vec{a})] \} &= \text{Tr}_{\mathfrak{h}} \{ (\mathbf{1}_x \otimes \mathbf{1}) U_{\vec{b}} F[H(\vec{a})] U_{\vec{b}} \} = \text{Tr}_{\mathfrak{h}} \{ (\mathbf{1}_x \otimes \mathbf{1}) F[-H(\vec{a})] \} \\ &= -\text{Tr}_{\mathfrak{h}} \{ (\mathbf{1}_x \otimes \mathbf{1}) F[H(\vec{a})] \} = 0, \end{aligned}$$

using that  $\mathbf{1}_x \otimes \mathbf{1}$  and  $U_{\vec{b}}$  commute. Inserting this into (A.7), we obtain

$$\mathrm{Tr}_{\mathfrak{h}}[(\mathbf{1}_x \otimes \mathbf{1})\gamma(\vec{a})] = \frac{1}{2} \mathrm{Tr}_{\mathfrak{h}}[\mathbf{1}_x \otimes \mathbf{1}] = 1, \quad (\text{A.8})$$

for any  $x \in \Lambda$ .

Next suppose that  $x, y \in \Lambda$ , set  $z = x - y$ , and use the unitary  $V_z := G^{|z|}\tau^z \otimes \mathbf{1} = \tau^z G^{|z|} \otimes \mathbf{1}$  and that

$$\begin{aligned} V_z F[H(\vec{a})] V_z^* &= F[G^{|z|} T G^{|z|} \otimes \mathbf{1} + \tau^z G \tau^{-z} \otimes (\vec{a} \cdot \vec{\sigma})] \\ &= F[(-1)^z T \otimes \mathbf{1} - (-1)^z G \otimes (\vec{a} \cdot \vec{\sigma})] \\ &= F[(-1)^z H(\vec{a})] = (-1)^z F[H(\vec{a})]. \end{aligned}$$

Since the Pauli matrices are traceless, we obtain

$$\begin{aligned} \mathrm{Tr}_{\mathfrak{h}}[(\mathbf{1}_x \otimes \vec{\sigma})\gamma(\vec{a})] &= \mathrm{Tr}_{\mathfrak{h}}\{(\mathbf{1}_x \otimes \vec{\sigma})F[H(\vec{a})]\} = \mathrm{Tr}_{\mathfrak{h}}\{(\mathbf{1}_y \otimes \vec{\sigma})V_z F[H(\vec{a})] V_z^*\} \\ &= -\mathrm{Tr}_{\mathfrak{h}}\{(\mathbf{1}_y \otimes \vec{\sigma})F[H(\vec{a})]\} = (-1)^{y-x} \mathrm{Tr}_{\mathfrak{h}}[(\mathbf{1}_y \otimes \vec{\sigma})\gamma(\vec{a})]. \end{aligned}$$

It follows that Inequalities (A.2) and (A.6) actually become *equalities* when we insert  $\gamma(\vec{a}) := \mathbf{1}[T \otimes \mathbf{1} - G \otimes (\vec{a} \cdot \vec{\sigma})]$  and  $\vec{w} := \vec{v}[\gamma(\vec{a})]$ . Choosing  $\vec{a} := g\Delta\vec{e}$ , this implies that

$$\frac{E_{\mathrm{HF}}(|\Lambda|)}{|\Lambda|} \leq \frac{\mathcal{E}_{\mathrm{HF}}(\gamma(g\Delta\vec{e}))}{|\Lambda|} = \frac{g}{2} + \mathcal{F}_L(\Delta^2)$$

and the asserted characterization (ii) of the Hartree–Fock ground states.

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