GENERALIZED HARTREE-FOCK THEORY AND THE HUBBARD MODEL

Volker Bach[(1)], Elliott H. Lieb[(2),(3)] and Jan Philip Solovej[(3)]

[(1)]*FB Mathematik, Technische Universität Berlin, Strasse des 17 Juni 136, D-10623 Berlin, Germany*
[(2)]*Department of Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, NJ, 08544*
[(3)]*Department of Mathematics, Fine Hall, Princeton University, Princeton, NJ, 08544*

Dedicated to Philippe Choquard on his sixty fifth birthday

Abstract: The familiar unrestricted Hartree-Fock variational principle is generalized to include quasi-free states. As we show, these are in one-to-one correspondence with the one-particle density matrices and these, in turn provide a convenient formulation of a generalized Hartree-Fock variational principle, which includes the BCS theory as a special case. While this generalization is not new, it is not well known and we begin by elucidating it. The Hubbard model, with its particle-hole symmetry, is well suited to exploring this theory because BCS states for the attractive model turn into usual HF states for the repulsive model. We rigorously determine the true, unrestricted minimizers for zero and for nonzero temperature in several cases, notably the half-filled band. For the cases treated here, we can exactly determine all broken and unbroken spatial and gauge symmetries of the Hamiltonian.

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I. INTRODUCTION

The Hubbard model has long been recognized as an interesting imitation of electron-electron interactions and of the correlations they induce. It also turns out, as we show here, that it is an interesting testing ground for Hartree-Fock (HF) theory, and it is one of the very few examples in many-body theory for which many properties of the *true*, energy minimizing HF ground state and pressure maximizing positive temperature state can be precisely elucidated without approximation, restriction or unjustified assumptions. (To avoid misunderstandings, we should make it clear at the outset that we consider only unrestricted HF theory.)

While studying the HF theory of the Hubbard model we were led to a critical study of HF theory itself—namely, the proper context in which to view it, as well as some of its very general features. This is the content of Sect. II which we can summarize as follows.

The usual HF theory for an N-particle system starts with a Slater determinant ψ formed from N orthonormal, one-particle functions of space and spin; the energy is then minimized with respect to the choice of these N functions. This ψ will generally break certain symmetries inherent in the original problem — typical examples being translation invariance and spin or spatial angular momenta. That being the case, it is not worse to permit a violation of particle-number conservation as well — if the energy can thereby be lowered. This is precisely what was done by Bardeen, Cooper and Schrieffer [BCS] in their theory of superconductivity. It is important, here to recall the simple fact that if a state violates a symmetry of the Hamiltonian (e.g. angular momentum, particle number) and if that state is then decomposed into its irreducible components, at least one component will have an energy no greater than (and often less than) the original state.

The proper Hilbert space, then, is Fock space, $\mathcal{F}$, the sum of all the original N-particle spaces with $N = 0, 1, 2, \ldots$. The simplest Hamiltonians on $\mathcal{F}$ are, of course, the quadratic ones, and they are all diagonalizable by Bogoliubov unitary transformations, which transforms creation operators $c^\dagger$ into linear combinations of c's and $c^\dagger$'s. In the context of fermionic theories, this transformation was discovered at the same time by Valatin [VJ] and Bogoliubov (see [BN]). The ground state of a quadratic Hamiltonian H^Q is a Bogoliubov transformation $\mathcal{U}$ applied to the vacuum (zero-particle state) $|0\rangle$. We call all such states of the form $\mathcal{U}|0\rangle$ a **generalized HF state** because the original N-particle determinant (which has the form $c_1^\dagger c_2^\dagger \ldots c_N^\dagger|0\rangle$ and which we call a **normal state**) is only the special case corresponding to an H^Q that contains terms of the form $c^\dagger c$ and N terms of the form $cc^\dagger$, but not the particle nonconserving terms cc or $c^\dagger c^\dagger$. Such generalized HF states, $\mathcal{U}|0\rangle$, are also called **quasi-free states** because they satisfy the conclusion of Wick's Theorem. Indeed, all quasi-free states are of this form, as we show below.

A generalized HF ground state is thus the ground state of some quadratic H^Q in Fock space. A positive temperature HF state is, likewise, the usual grand canonical Gibbs state for such an H^Q. In analogy with the ground state, such a grand canonical Gibbs state is called **normal** when H^Q is particle conserving. For the ground state, the H^Q is determined so that the expectation value of the original many-body Hamiltonian, H, of our system is as small as possible. For positive temperatures, H^Q is chosen (in a temperature dependent way) to maximize the pressure in the grand canonical ensemble.

The paired (BCS) state, which is so important in superconductivity theory, is also of the form $\mathcal{U}|0\rangle$, a Bogoliubov transformation of the vacuum. Thus, normal HF theory and BCS theory are but two aspects of the same general theory: find the best substitute quadratic Hamiltonian or, equivalently, find the best Bogoliubov transformation. This relationship was certainly known [BN], [dG], [BR], [DJK], but our personal experience is that it is far from being universally appreciated. At first it seems surprising that one-particle states can somehow evolve into pair states, and the explanation is roughly the following: It is always true that for each mode α, $\mathcal{U}c_\alpha^\dagger\mathcal{U}^\dagger = d^\dagger + e$, where $d^\dagger$ (resp. e) is proportional to a creation (resp. annihilation) operator, but it is possible that $d^\dagger = 0$ or $e = 0$. If $d^\dagger = 0$ then $\psi = \mathcal{U}|0\rangle$ contains the mode $e^\dagger$, i.e., $e^\dagger e\psi =$ (pos. const)ψ. If $e = 0$, ψ just contains a factor proportional to $|0\rangle$, i.e., $d\psi = 0$. If e and $d^\dagger$ are both nonvanishing then such modes must come in pairs (as we prove in Theorem 2.2) and ψ is found to contain a pairing factor $(1 + d^\dagger e^\dagger)$ acting on $|0\rangle$. Alternatively, it turns out that to every eigenvalue 1 of the particle conserving part, γ, of the one-particle density matrix (1-*pdm*), Γ, associated with the state $\psi = \mathcal{U}|0\rangle$ there corresponds a simple one-particle state in ψ, but to every eigenvalue of γ between 0 and 1 there corresponds a pair state in ψ.

The 1-*pdm* plays an essential structural mathematical role in HF theory. The set of quasi-free states (generalized or not) does not have a linear or convex structure. A linear or convex combination of such states is not necessarily a quasi-free state. However, a convex combination of 1-*pdms* is a 1-*pdm*, i.e., $\Gamma = \lambda\Gamma_1 + (1-\lambda)\Gamma_2$ is a 1-*pdm* if $0 \leq \lambda \leq 1$ and Γ_1 and Γ_2 are 1-*pdms*. This fact allows us to compensate for the missing convex structure of quasi-free states. Thus given $\psi_{1,2} = \mathcal{U}_{1,2}|0\rangle$ with $\mathcal{U}_{1,2}$ being two Bogoliubov transformations, we can form the 1-*pdms* Γ_1 and Γ_2 and then form Γ as above. Finally, we can return to the level of the quasi-free states and thereby define a quasi-free state that interpolates between the two original states. Sect. II contains a detailed description of quasi-free states, density matrices and quadratic Hamiltonians.

We present this partly for the reader's convenience, but also because we could not find quite what we need in the literature on quasi-free states (which usually concentrates on quasi-free states in terms of algebraic automorphisms rather than operators) or in the excellent book by Blaizot and Ripka [BR] which does not deal explicitly with the infinite dimensional Hilbert space $L^2(\mathbf{R}^3)$, the space of square integrable functions on $\mathbf{R}^3$, needed for our other theorems in Sect. II on atomic HF theory.

The notation in Sect. II is a bit complicated and one reason for this is the necessity to introduce antiunitary transformations (because c's transform by antiunitaries if $c^\dagger$'s transform by unitaries). Consequently, if one tries to write equations in a basis independent way, one needs more than the usual notation of linear operator theory. If one fixes a basis, however, one can use the ordinary linear operator notation, but then complex conjugates (denoted by superscript bars) and indices appear in profusion. We have opted for the second route.

The general Theorem 2.14 in Sect. II about the usual (N-particle) HF theory should have been well known but seemingly was not. It applies to repulsive two-body potentials (as in the real world of electrons with Coulomb interaction) and states two things. The first is that the N one-particle states are precisely the energetically *lowest* eigenvectors of the HF operator. (This fact was stated in [LS], and the proof was sketched in [LE4]). While the N HF orbitals are distinct eigenvectors of the HF operator, it is not obvious, a priori, that they are the lowest ones; indeed, this might not be true when the interactions are attractive. The second part is surprising, for its conclusion runs counter to what one might naively assume. *There are never unfilled shells* (for any choice of N). That is to say, the degeneracy of the last level of the HF operator is *always* precisely what is needed to accommodate the available number of electrons — not more than that!

Readers who are already familiar with the formalities of Sect. II are advised to skip over it and to turn to Sect. III, which contains the HF analysis of the attractive Hubbard model. It beautifully illustrates the relationship between BCS and normal states discussed above. It is well known that a particle-hole transformation (on the down spins alone) converts the repulsive and the attractive models into each other. What does this do to generalized HF states? The answer, simply, is that a normal HF state may be turned into a BCS state (in which there is pure pairing without isolated one-particle states). Indeed, it turns out that the repulsive Hubbard model at half-filling (i.e., the expected particle number equals $|\Lambda|$, the number of sites in Λ) always has a normal state as its optimal state (for zero and for positive temperature). The attractive model at half-filling then has a BCS state (and, when the lattice is bipartite, also a normal state of the same energy) as its ground state. This was well understood by Dichtel *et. al.* [DJK], but they did not prove that their state was, indeed, the true minimum energy HF state. We do so here as a special case of our results in Sects. III and IV.

At the outset we emphasize that translation invariance is not assumed. By the word "lattice" we mean a collection of points connected by bonds (or edges). Perhaps "graph" would be more accurate, but physicists are accustomed to the word lattice. If our lattice does have translation invariance, e.g. a hypercubic lattice, we shall say so explicitly. We do, in fact, investigate translation invariant cases and we do discuss the cases in which the translation invariance is broken by the HF state. Thus, there is a special column in the tables of Sect. V for lattices that have the additional property of translation invariance (or some other spatial symmetry). In any case, our systems are always finite.

Among the things we can prove about HF theory for a bipartite lattice is the existence of a phase transition from a BCS state at low temperature to a normal state at high temperature.

Sect. IV contains the analysis of the repulsive Hubbard model; most of the results here—but not all—are a transcription of the results in Sect. III via a particle-hole transformation. One of the earliest HF studies of this model was by Penn [PD].

One question that is peculiar to unrestricted HF theory is whether or not the orbitals (which are well defined even for the generalized, particle nonconserving theory) are simple products of spatial functions and spin functions (the latter being one of two types, either spin up $\uparrow$ or spin down $\downarrow$). For the half-filled band and real hopping matrices we can show this to be true for both the attractive and repulsive models; this is one of our more complicated proofs, and it involves a somewhat delicate convexity argument.

Another question concerns the uniqueness of the HF state for a finite system. Apart from possible global gauge transformations (those describes as "broken" in Tables 1–3 in Sect. V) uniqueness does hold for a half-filled band as we prove in Theorems 3.12 and 4.5.

The main thing one wishes to know about the true HF state is whether or not it is qualitatively correct. From that point of view, a main question is whether the HF state breaks the symmetries of the problem, and if it does so in conformity with what one believes to be the case in the corresponding exact quantum state. For example, the repulsive Hubbard model on a bipartite lattice has total spin equal to $\big||A| - |B|\big|$ (where $|A|$ and $|B|$ are the number of sites in the two sublattices) in a finite system ground state [LE2] (see also [LE3]) and is expected to have Neél long range order in three or more dimensions. This Neél state *partially* breaks the original translation invariance of the Hamiltonian (if there is any to start with) into a smaller group consisting of translations on each sublattice separately. This is exactly what we prove to be the case for the HF ground or Gibbs state. Indeed, after a suitable rotation of the spin basis, we will find the spins to point upward on the A-sublattice and downward on the B-sublattice This validates the predictions of mean field calculations for the translation invariant case in the physics literature [DJK], [CM], [FE]. As far as we know, this self-consistent antiferromagnetic A-B spin structure was assumed to be valid in the energy minimizing ground state, but it was never proved that this was indeed true. In principle, some sort of further symmetry breaking could occur. Our results show that this does not happen.

Sect. V summarizes what we can prove about the breaking of symmetry in different cases. Unfortunately, different combinations of conditions have to be treated separately; the basic possible postulates are bipartite (or non-bipartite) lattice, real (or complex) hopping matrix, repulsive or attractive interaction, half-filled (or not half-filled) band, translation invariance (or no invariance). The symmetries to be investigated are spin $SU(2)$, pseudospin $SU(2)$, $U(1)$ (particle conservation) $\mathbf{Z}_2$ (particle-hole symmetry) and translation invariance. For the reader's convenience, our conclusions are encapsulated in three tables.

The phrase "symmetry breaking" does require a precise definition and we supply that in Sect. V. To us it means that the state fails to have the symmetry that the Hamiltonian has. Some authors, e.g., [BR] use a more restrictive definition, namely that the state also fails to belong to exactly one irreducible representation of the symmetry group. For example, the completely magnetized ground state of a Heisenberg ferromagnet breaks rotation symmetry in our sense, but not in the restrictive sense. As a matter of experience, however, this case is rare, i.e., usually the two senses agree in practice. At least this is so in the cases we can analyze completely here. In any event, as explained in Sect. IV, the restrictive definition requires a linear structure and, therefore, is not appropriate for HF theory.

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II. DEFINITION AND PROPERTIES OF GENERALIZED HF STATES

Since its introduction in 1930 the notion of a Hartree-Fock ground state and positive temperature state has evolved. Our purpose in this section is to state clearly several definitions of these states, demonstrate their equivalence and prove some of their fundamental properties. Despite years of attention to the subject it is surprising that some of the basic properties have not been clearly stated, much less proved. Two of these are in Theorem 2.12 (the variational principle [LE1]) and Theorem 2.14, which states that there are *never* unfilled shells, regardless of the particle number.

II.a DEFINITIONS OF HF STATES

The original point of view was that a HF state is a single determinant of one-particle orbitals, in the variables $z_1, z_2, \ldots, z_N$, where $z = (x, \sigma)$ denotes a space-spin variable for one particle. The inner product of two functions is $\langle \varphi_1 | \varphi_2 \rangle = \sum_\sigma \int \overline{\varphi_1} \varphi_2(x, \sigma) dx$. The usual HF state is then

$$\psi_{\mathrm{HF}} = (N!)^{-1/2} \mathrm{Det}[\varphi_i(x_j)]_{1 \le i,j \le N} =: (N!)^{-1/2} (\varphi_1 \wedge \ldots \wedge \varphi_N), \tag{2a.1}$$

in which $\mathrm{Det}[\langle \varphi_i | \varphi_j \rangle] = 1$.

This is not general enough for our purposes because we also want to allow for HF states in which the particle number is not conserved. After all, there are other quantities such as total spin, total momentum and total angular momentum that are not necessarily sharp in a HF state, and there is no reason why the particle number should not suffer a similar fate. In any case, when we go to positive temperature, the HF state should not be expected to be a pure state if it is to have any physical relevance. For these reasons we are going to make definitions that go beyond simple determinants. There is nothing new about the definitions given here but it is important for us to be very clear about them.

Abstractly we begin with a one-particle Hilbert space $\mathcal{H}$ (finite or infinite dimensional, but always separable). We define the fermionic N-particle space to be the antisymmetric tensor product of $\mathcal{H}^{(N)} := \overbrace{\mathcal{H} \wedge \ldots \wedge \mathcal{H}}^{N \text{ times}}$ for all $N = 1, 2, 3 \ldots$. A **simple vector** in $\mathcal{H}^{(N)}$ is of the form

$$f_1 \wedge f_2 \wedge \ldots \wedge f_N := \sum_{\text{permutations}} (-)^\pi \cdot f_{\pi(1)} \otimes f_{\pi(2)} \otimes \ldots \otimes f_{\pi(N)}, \tag{2a.2}$$

where each f_i is in $\mathcal{H}$. A general vector in $\mathcal{H}^{(N)}$ is a (possibly infinite) linear combination of such simple vectors. We note that the squared norm of the above simple vector is†

$$\langle f_1 \wedge \ldots \wedge f_N \big| f_1 \wedge \ldots \wedge f_N \rangle = N! \ \mathrm{Det}[\langle f_i | f_j \rangle]_{1 \le i,j \le N}. \tag{2a.3}$$

With the identification $\mathcal{H}^{(1)} = \mathcal{H}$ and $\mathcal{H}^{(0)} = \mathbf{C} \cdot |0\rangle$ where $|0\rangle$ is the vacuum and $\langle 0|0\rangle := 1$ (of course, $|0\rangle \notin \mathcal{H}$), we can define the Fock Hilbert space

$$\mathcal{F} := \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)} \oplus \mathcal{H}^{(2)} \oplus \ldots. \tag{2a.4}$$

† Dirac notation will be used. $\langle f|g\rangle$ is the inner product of f and g, which is linear in g and conjugate linear in f. $\langle f|A|g\rangle = \langle f|Ag\rangle$ is the inner product of f with the vector Ag, i.e., the operator A acts to the right. It is important to keep this in mind when A is not self-adjoint.

To any vector $f \in \mathcal{H}$ we associate a creation operator $c^\dagger(f)$ and an annihilation operator $c(f)$, each acting on $\mathcal{F}$. The creation operator acts on simple vectors by

$$c^\dagger(f)(f_1 \wedge \ldots \wedge f_N) = (N+1)^{-1/2}(f \wedge f_1 \wedge \ldots \wedge f_N). \tag{2a.5}$$

This definition extends to $\mathcal{F}$ by linearity, and $c(f)$ is defined to be the adjoint operator of $c^\dagger(f)$. Note that $c(f)|0\rangle = 0$ and that $c(\lambda f) = \overline{\lambda} c(f)$ for any $f \in \mathcal{H}$ and any $\lambda \in \mathbf{C}$. (Here and elsewhere complex conjugation is denoted by a bar.) By this construction the creation and annihilation operators fulfill the canonical anticommutation relations (CAR):

$$\begin{aligned} \{c(f), c^\dagger(g)\} &:= c(f)c^\dagger(g) + c^\dagger(g)c(f) = \langle f|g\rangle \cdot \mathbf{1}, \\ \{c^\dagger(f), c^\dagger(g)\} &= \{c(f), c(g)\} = 0. \end{aligned} \tag{2a.6}$$

Here, $\mathbf{1}$ is the identity operator on $\mathcal{F}$. We remark that the Fock space $\mathcal{F}$ is determined by the vacuum $|0\rangle$ and a complete set of operators $c^\dagger(f), c(f)$ that obey the CAR. Indeed, simple vectors can be written as

$$f_1 \wedge \ldots \wedge f_N = (N!)^{1/2} c^\dagger(f_1)c^\dagger(f_2)\ldots c^\dagger(f_N)|0\rangle. \tag{2a.7}$$

A **Bogoliubov transformation** of $\mathcal{F}$ is a unitary operator $\mathcal{W}$, on $\mathcal{F}$, with the following special property: For each vector $f \in \mathcal{H}$

$$d^\dagger(f) := \mathcal{W} c^\dagger(f) \mathcal{W}^\dagger = c^\dagger(g) + c(h) = c^\dagger(\widehat{u}f) + c(\widehat{v}f). \tag{2a.8}$$

Here g and h are vectors in $\mathcal{H}$ and, by the linearity of $\mathcal{W}$ we see that there must exist a linear operator $\widehat{u}$ on $\mathcal{H}$ such that $g = \widehat{u}f$ and there must exist an antilinear operator $\widehat{v}$ on $\mathcal{H}$ such that $h = \widehat{v}f$ (antilinear means that $\widehat{v}(\lambda a + b) = \overline{\lambda}\widehat{v}(a) + \widehat{v}(b)$). It is easy to check that the unitarity of $\mathcal{W}$, which in particular implies the CAR for the operators $d^\dagger(f), d(f)$, results in certain conditions on $\widehat{u}$ and $\widehat{v}$. Because $\widehat{v}$ is antilinear these are not easy to state. One way is to choose an orthonormal basis $f_1, f_2, \ldots$ in $\mathcal{H}$ and define the matrix elements $v_{ij} = \langle f_i|\widehat{v}f_j\rangle$ and $u_{ij} = \langle f_i|\widehat{u}f_j\rangle$. In terms of the linear operators u and v having the same matrix elements the condition is that the linear operator

$$W = \begin{pmatrix} u & v \\ \overline{v} & \overline{u} \end{pmatrix}, \tag{2a.9}$$

acting on $\mathcal{H} \oplus \mathcal{H}$, is a unitary matrix. Here $\overline{u}, \overline{v}$ denote the linear operators with the complex conjugate matrix elements $\overline{u}_{ij}, \overline{v}_{ij}$. An equivalent, basis independent statement is this: to every antilinear operator $\widehat{v}$ we can always associate an antilinear operator $\widehat{v}^T$ such that $\langle f|\widehat{v}g\rangle = \overline{\langle \widehat{v}^T f|g\rangle}$ for every $f, g \in \mathcal{H}$. The condition becomes

$$\begin{aligned} \widehat{u}^\dagger\widehat{u} + \widehat{v}^T\widehat{v} &= \mathbf{1} = \widehat{u}\widehat{u}^\dagger + \widehat{v}\widehat{v}^T \\ \widehat{v}^T\widehat{u} + \widehat{u}^\dagger\widehat{v} &= 0 = \widehat{u}\widehat{v}^T + \widehat{v}\widehat{u}^\dagger \end{aligned} \tag{2a.10}$$

In case $\mathcal{H}$ is finite dimensional the converse is also true, i.e., if a pair $(\widehat{u}, \widehat{v})$ satisfies (2a.10) then there is a unique unitary operator $\mathcal{W}$ on $\mathcal{F}$ satisfying (2a.8). If $\mathcal{H}$ is infinite dimensional it may not be possible to find a $\mathcal{W}$, even if (2a.10) is true. This phenomenon occurs, for example, when $\widehat{u} = 0$. A sufficient condition for the existence of $\mathcal{W}$ is given in Theorem 2.2.

The second notion needed for generalized HF theory is a quasi-free state. In general a state, ρ, on the set of bounded operators that act on $\mathcal{F}$ is a (complex-valued) linear map (i.e., for all operators

A and B, $\quad \rho(\lambda A+B) = \lambda\rho(A)+\rho(B)$) satisfying the conditions $\rho(\mathbf{1}) = 1$ and $\rho(A^\dagger A) \geq 0$ (which implies $\overline{\rho(A)} = \rho(A^\dagger)$). The example that will concern us most is a **pure state** $\rho(A) = \langle\psi|A\psi\rangle$ for some $\psi \in \mathcal{F}$. Another important example is the **Gibbs state** $\rho(A) = Z^{-1}\mathrm{Tr}[A\exp(-\beta H)]$ with $Z = \mathrm{Tr}[\exp(-\beta H)]$ for some Hamiltonian H on $\mathcal{F}$ with $Z < \infty$.

A state ρ is **quasi-free** if all correlation functions can be computed from Wick's Theorem, i.e., if the operators $e_1, e_2, \ldots, e_{2N}$ are each either a $c^\dagger$ or a c, then $\rho(e_1 e_2 \ldots e_{2N-1}) = 0$ and

$$\rho(e_1 e_2 \ldots e_{2N}) = \sum_\pi{}' (-)^\pi \rho(e_{\pi(1)}e_{\pi(2)}) \ldots \rho(e_{\pi(2N-1)}e_{\pi(2N)}) \tag{2a.11}$$

where $\sum'_\pi$ is the sum over permutations π which satisfy $\pi(1) < \pi(3) < \ldots < \pi(2N-1)$ and $\pi(2j-1) < \pi(2j)$ for all $1 \leq j \leq N$. The right side of (2a.11) is also known as the Pfaffian of the triangular array $[\rho(e_i e_j)]_{1\leq i<j\leq 2N}$. In particular, we have the important formula

$$\rho(e_1e_2e_3e_4) = \rho(e_1e_2)\rho(e_3e_4) - \rho(e_1e_3)\rho(e_2e_4) + \rho(e_1e_4)\rho(e_2e_3). \tag{2a.12}$$

When this is applied later to the expectation value of the two-body potential these terms will correspond to the direct, the exchange and the pairing energies (see (2c.8)).

We remark that the quasi-free states are invariant under Bogoliubov transformations, i.e., if ρ is quasi-free and $\mathcal{W}$ is a Bogoliubov transformation, then the state $\rho_\mathcal{W}(A) := \rho(\mathcal{W}A\mathcal{W}^\dagger)$ is quasi-free, too.

If ρ is a pure state, i.e., $\rho(A) = \langle\psi|A|\psi\rangle$, and if the vector ψ lies solely in some fixed $\mathcal{H}^{(N)}$ (including the possibility $N = 0$) then ρ is a quasi-free state if and only if ψ is a normalized *simple* vector (including the possibility $\psi = |0\rangle$). This state is *the usual N-particle Slater determinant state* defined by taking expectation values with respect to the vector ψ_{HF} given in (2a.1).

We can define the (unbounded) particle **number operator** on $\mathcal{F}$ by the formal sum

$$\mathcal{N} = \sum_{N=0}^\infty N\Pi^{(N)}, \tag{2a.13}$$

where $\Pi^{(N)}$ is the projector onto the subspace $\mathcal{H}^{(N)} \subset \mathcal{F}$. (Note that $\mathbf{1} = \sum_N \Pi^{(N)}$.) A state ρ **has finite particle number** if

$$\rho(\mathcal{N}) := \sum_{N=0}^\infty N\rho(\Pi^{(N)}) \tag{2a.14}$$

is finite. These are the states of primary physical interest.

A **generalized Hartree-Fock state** *is defined to be any quasi-free state having finite particle number.*

II.b ONE-PARTICLE DENSITY MATRICES

Let ρ be a state and let $\{f_1, f_2, \ldots\}$ be an orthonormal basis in $\mathcal{H}$. We define the one-particle density matrix (1-*pdm*) Γ to be the self-adjoint operator on $\mathcal{H}\oplus\mathcal{H}$ whose matrix elements are

$$\left\langle \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \middle| \Gamma \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \right\rangle = \rho\left(\left[c^\dagger(g_1) + c(\overline{g}_2)\right]\left[c(h_1) + c^\dagger(\overline{h}_2)\right]\right), \tag{2b.1}$$

where $\overline{g} := \sum_k \overline{\mu}_k f_k$ when $g = \sum_k \mu_k f_k$. Note the ordering of the operators here. The matrix $\mathbf{1} - \Gamma$ has a more "natural" appearance; using the CAR we find that

$$\left\langle \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \,\middle|\, (\mathbf{1} - \Gamma) \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \right\rangle = \rho\big([c(h_1) + c^\dagger(\overline{h}_2)][c^\dagger(g_1) + c^\dagger(\overline{g}_2)] \big). \tag{2b.2}$$

Note that the definition of Γ as an operator on $\mathcal{H} \oplus \mathcal{H}$ depends on the choice of the basis $\{f_1, f_2, \ldots\}$. If this basis is changed then Γ itself changes if the antiunitary map $g \mapsto \overline{g}$ changes (which may or may not occur). The underlying reason that Γ cannot be defined in a basis independent way is that Γ is not, intrinsically, a linear map on $\mathcal{H} \oplus \mathcal{H}$; it also has an antilinear component. This basis dependence is the price we pay for avoiding the introduction of an abstract antiunitary map. The quantities we are going to compute later by means of the 1-*pdm* Γ will, however, be independent of the choice of the basis $\{f_1, f_2, \ldots\}$, which we shall consider to be fixed henceforth.

2.1 LEMMA: *For any state ρ and any orthonormal basis $\{f_1, f_2, \ldots\}$*

$$0 \le \Gamma \le \mathbf{1} \tag{2b.3}$$

holds as an operator on $\mathcal{H} \oplus \mathcal{H}$.

Proof: Let $\varphi = (f, g) \in \mathcal{H} \oplus \mathcal{H}$ be normalized. Then $1 = \|\varphi\|^2 = \|f\|^2 + \|g\|^2 = \|f\|^2 + \|\overline{g}\|^2$ and, from (2b.1) and the CAR, it follows that

$$\begin{aligned} 0 \le \langle \varphi | \Gamma \varphi \rangle &= \rho\big[(c^\dagger(f) + c(\overline{g}))(c(f) + c^\dagger(\overline{g})) \big] \\ &= (\|f\|^2 + \|\overline{g}\|^2)\rho(\mathbf{1}) - \rho\big[(c(f) + c^\dagger(\overline{g}))(c^\dagger(f) + c(\overline{g})) \big] \le 1. \quad \blacksquare \end{aligned} \tag{2b.4}$$

It is convenient to view Γ as a 2×2-matrix of operators on $\mathcal{H}$. Writing

$$\Gamma =: \begin{pmatrix} \gamma & \alpha \\ \alpha^\dagger & 1 - \overline{\gamma} \end{pmatrix} \tag{2b.5}$$

one easily finds, using $c_k^\dagger := c^\dagger(f_k)$, that

$$\begin{aligned} \langle f_m | \gamma f_k \rangle &= \rho(c_k^\dagger c_m), \\ \langle f_m | \alpha^\dagger f_k \rangle &= \rho(c_k^\dagger c_m^\dagger), \end{aligned} \tag{2b.6}$$

where the operator $\overline{A}$ is defined by

$$\langle f_m | \overline{A} f_k \rangle := \overline{\langle f_m | A f_k \rangle}. \tag{2b.7}$$

Note that

$$\gamma^\dagger = \gamma, \quad \alpha^T = -\alpha \tag{2b.8}$$

(where $\alpha^T := \overline{\alpha^\dagger}$).

In view of (2a.11) and the density of polynomials in the algebra of observables, the 1-*pdm* Γ of a quasi-free state ρ uniquely determines ρ. More importantly, any Γ is the 1-*pdm* of a quasi-free state ρ, as we shall show in Theorem 2.3 below. We shall, however, restrict attention to finite particle states. It is easily seen that $\mathcal{N} = \sum_k c_k^\dagger c_k$ and that, for any state,

$$\rho(\mathcal{N}) = \sum_k \rho(c_k^\dagger c_k).$$

First, we give the relationship between the 1-*pdm* Γ of a state ρ and the 1-*pdm* $\Gamma_{\mathcal{W}}$ of the transformed state $\rho_{\mathcal{W}}$, $\rho_{\mathcal{W}}(A) := \rho(\mathcal{W}A\mathcal{W}^\dagger)$, assuming $\mathcal{W}$ is a Bogoliubov transformation. Using (2a.9) we can write the Bogoliubov transformation (2a.8) as

$$\begin{pmatrix} d_k \\ d_k^\dagger \end{pmatrix} = \sum_i \begin{pmatrix} u_{ki}^\dagger & \overline{v}_{ki}^\dagger \\ v_{ki}^\dagger & \overline{u}_{ki}^\dagger \end{pmatrix} \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix} =: \sum_i (W^\dagger)_{ki} \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix}. \tag{2b.9}$$

Note, as indicated above, that each $(W^\dagger)_{ki}$ is a 2×2 matrix. We then find that

$$(\mathbf{1} - \Gamma_{\mathcal{W}})_{kl} = \begin{pmatrix} \rho(d_k d_l^\dagger) & \rho(d_k d_l) \\ \rho(d_k^\dagger d_l) & \rho(d_k^\dagger d_l) \end{pmatrix} = \sum_{i,j} (W^\dagger)_{ki} (\mathbf{1} - \Gamma)_{ij} (W)_{jl}. \tag{2b.10}$$

Thus

$$\Gamma_{\mathcal{W}} = W^\dagger \Gamma W. \tag{2b.11}$$

We now give a sufficient condition for the operator W in (2a.9) to represent a Bogoliubov transformation in $\mathcal{F}$.

2.2 THEOREM: *Any unitary operator W of the form (2a.9) that satisfies the condition* $\mathrm{Tr}[vv^\dagger] < \infty$ *always corresponds to a Bogoliubov transformation $\mathcal{W}$ on $\mathcal{F}$ with*

$$d^\dagger(f) := \mathcal{W} c^\dagger(f) \mathcal{W}^\dagger = c^\dagger(uf) + c(v\overline{f}). \tag{2b.12}$$

Moreover, $\mathcal{W}|0\rangle = |\psi\rangle$ is the state

$$|\psi\rangle = \prod_i \left\{ (1 - \zeta_i)^{1/2} + \zeta_i^{1/2} c^\dagger(h_i) c^\dagger(k_i) \right\} \prod_{i=1}^r c^\dagger(g_i)|0\rangle. \tag{2b.13}$$

Here, $\zeta_1, \zeta_2, \ldots,$ denote the eigenvalues of $vv^\dagger$ in the interval (0,1) counted with half their multiplicity (these eigenvalues are all evenly degenerate), and r is the multiplicity of 1 as an eigenvalue of $vv^\dagger$. The vectors $g_1, g_2, \ldots, g_r, h_1, k_1, h_2, k_2, \ldots$ form an orthonormal family of eigenvectors of $vv^\dagger$ with $g_1, g_2, \ldots, g_r$ being the eigenvectors of eigenvalue 1. The pair of vectors h_i, and $k_i := (\zeta_i - \zeta_i^2)^{-1/2} u\overline{v}^\dagger \overline{h}_i$ are eigenvectors of $vv^\dagger$ of eigenvalue ζ_i.

Remark: We refer the reader to [AH] where the first statement of the lemma, together with its converse (which is not needed here), is proved ([AH], Theorem 7). However, we are not aware that the explicit formula (2.22), which we do require, is readily accessible.

Proof: The unitarity of the operator W implies the following conditions similar to (2a.10) for the linear operators u and v:

$$\begin{aligned} u^\dagger u + \overline{v}^\dagger \overline{v} = \mathbf{1} = uu^\dagger + vv^\dagger \\ \overline{v}^\dagger \overline{u} + u^\dagger v = 0 = u\overline{v}^\dagger + v\overline{u}^\dagger. \end{aligned} \tag{2b.14}$$

Thus, $0 \leq vv^\dagger \leq \mathbf{1}$ as an operator on $\mathcal{H}$ with purely discrete spectrum, thanks to $\mathrm{Tr}[vv^\dagger] < \infty$. Furthermore, if h is a normalized eigenvector of $vv^\dagger$ with eigenvalue $0 < \zeta < 1$ we find, using (2b.14), that $k = (\zeta - \zeta^2)^{-1/2} u\overline{v}^\dagger \overline{h}$ satisfies

$$\begin{aligned} vv^\dagger k &= (\zeta - \zeta^2)^{-1/2} vv^\dagger u\overline{v}^\dagger \overline{h} = -(\zeta - \zeta^2)^{-1/2} v\, \overline{u}^\dagger \overline{v}\, \overline{v}^\dagger \overline{h} \\ &= -\zeta(\zeta - \zeta^2) v\overline{u}^\dagger \overline{h} = \zeta k \end{aligned} \tag{2b.15}$$

and thus k is also an eigenvector of $vv^\dagger$. Moreover,

$$\begin{aligned} \langle h \mid k \rangle &= (\zeta - \zeta^2)^{-1/2} \langle h \mid u\overline{v}^\dagger \overline{h} \rangle = -(\zeta - \zeta^2) \langle h \mid v\overline{u}^\dagger \overline{h} \rangle \\ &= -(\zeta - \zeta^2) \langle \overline{u} v^\dagger h \mid \overline{h} \rangle = -\langle h \mid k \rangle \end{aligned} \tag{2b.16}$$

and hence $\langle h \mid k \rangle = 0$. Likewise, we see that $\langle k \mid k \rangle = 1$. Iterating the map from h to k will not produce more eigenvectors since $(\zeta - \zeta^2)^{-1/2} u\overline{v}^\dagger \overline{k} = (\zeta - \zeta^2)^{-1} u\overline{v}^\dagger \overline{u} v^\dagger h = (\zeta - \zeta^2)^{-1} uu^\dagger vv^\dagger h = -h$.

We can thus find an orthonormal basis for $\mathcal{H}$ of the form $g_1, \ldots, g_r, h_1, k_1, h_2, k_2, \ldots, l_1, l_2, \ldots$, where $g_1, g_2, \ldots$ and $l_1, l_2, \ldots$ are the eigenvectors of $vv^\dagger$ of eigenvalue 1 and 0, respectively. Another orthonormal basis is given by $\overline{v}^\dagger \overline{g}_1, \ldots, \overline{v}^\dagger \overline{g}_r, \zeta_1^{-1/2} \overline{v}^\dagger \overline{h}_1, \zeta_1^{-1/2} \overline{v}^\dagger \overline{k}_1, \ldots, u^\dagger \overline{l}_1, u^\dagger \overline{l}_2, \ldots$. To prove this we first note, as is easily seen, that this is an orthonormal family. We then note that if $f \in \mathcal{H}$ is orthogonal to all members of this family then $\overline{v}^\dagger \overline{v} f = 0$ (because $\overline{v} f$ is orthogonal to $\overline{g}_1, \ldots, \overline{g}_r, \overline{h}_1, \overline{k}_1, \ldots$ but not necessarily to $\overline{l}_1, \ldots$; however $\overline{v}^\dagger$ annihilates $\overline{l}_1, \ldots$). Hence $v^\dagger u f = -\overline{u}^\dagger \overline{v} f = 0$. Thus uf is an eigenvector for $vv^\dagger$ of eigenvalue 0, i.e., $uf \in \mathrm{span}\{l_1, l_2, \ldots\}$, but then $f = (1 - \overline{v}^\dagger \overline{v}) f = u^\dagger u f \in \mathrm{span}\{u^\dagger l_1, u^\dagger l_2, \ldots\}$, and thus $f = 0$.

Using this latter basis we define, in agreement with (2b.12),

$$d(\overline{v}^\dagger \overline{g}_i) := c(u\overline{v}^\dagger \overline{g}_i) + c^\dagger(vv^\dagger g_i) = c^\dagger(g_i) \quad i = 1, \ldots, r, \tag{2b.17}$$

where we have used $u\overline{v}^\dagger \overline{g}_i = -v\overline{u}^\dagger \overline{g}_i = 0$, which follows from $uu^\dagger g_i = (\mathbf{1} - vv^\dagger) g_i = 0$. We also make the definitions, for $i = 1, 2, \ldots$,

$$d(\zeta_i^{-1/2} \overline{v}^\dagger \overline{h}_i) := \zeta_i^{-1/2} c(u\overline{v}^\dagger \overline{h}_i) + \zeta_i^{-1/2} c^\dagger(vv^\dagger h_i) = (1 - \zeta_i)^{1/2} c(k_i) + \zeta_i^{1/2} c^\dagger(h_i), \tag{2b.18}$$

$$d(\zeta_i^{-1/2} \overline{v}^\dagger \overline{k}_i) := \zeta_i^{-1/2} c(u\overline{v}^\dagger \overline{k}_i) + \zeta_i^{-1/2} c^\dagger(vv^\dagger k_i) = -(1 - \zeta_i)^{1/2} c(h_i) + \zeta_i^{1/2} c^\dagger(k_i), \tag{2b.19}$$

$$d(u^\dagger l_i) := c(uu^\dagger l_i) + c^\dagger(v\overline{u}^\dagger \overline{l}_i) = c(\overline{l}_i). \tag{2b.20}$$

We shall now show that (2b.13) defines a normalized vector $|\psi\rangle$ in $\mathcal{F}$ annihilated by all the operators in (2b.18–20). To show that the somewhat formal expression on the right side in (2b.13) defines a vector in $\mathcal{F}$ we expand the (possibly infinite) product, thereby arriving at a (possibly infinite) sum of (possibly infinite) products. Each term in this sum that contains a product of infinitely many $c^\dagger$'s is zero since it will also contain a product of infinitely many $\zeta_i^{1/2}$, and $\zeta_i \to 0$ as $i \to \infty$. Hence, the sum is at most a countable sum of orthogonal simple vectors in $\mathcal{F}$. An appropriate truncation of this sum gives

$$|\psi_N\rangle := \prod_{i>N} (1 - \zeta_i)^{1/2} \prod_{i \leq N} [(1 - \zeta_i)^{1/2} + \zeta_i^{1/2} c^\dagger(h_i) c^\dagger(k_i)] \prod_{i=1}^{r} c^\dagger(g_i) |0\rangle. \tag{2b.22}$$

We note that $\langle \psi_N \mid \psi_N \rangle = \prod_{i>N}(1-\zeta_i) \geq 1 - \sum_{i>N}\zeta_i$, which is non-zero and converges to 1 as $N \to \infty$ since $\sum_i \zeta_i < \infty$. If $M > N$ then $|\psi_N\rangle$ is orthogonal to $|\psi_M - \psi_N\rangle$ and

$$\langle \psi_M - \psi_N \mid \psi_M - \psi_N \rangle = \langle \psi_M \mid \psi_M \rangle - \langle \psi_N \mid \psi_N \rangle = \prod_{i>M}(1-\zeta_i) - \prod_{i>N}(1-\zeta_i) \to 0 \qquad (2b.23)$$

as $M \to \infty$. Hence there is a normalized $|\psi\rangle \in \mathcal{F}$ such that $|\psi_N\rangle \to |\psi\rangle$ as $N \to \infty$. It is easy to check that any operator in the list (2b.18–20) will annihilate $|\psi_N\rangle$ if N is large enough. Thus $|\psi\rangle$ is annihilated by all the operators in (2b.18–20), and hence by any operator $d(f) := c^\dagger(uf) + c(v\overline{f})$.

Denoting $d_k^\dagger := c^\dagger(uf_k) + c(vf_k)$ (recall $\overline{f}_k = f_k$) we define $\mathcal{W} : \mathcal{F} \to \mathcal{F}$ by

$$\mathcal{W} c_1^\dagger \ldots c_n^\dagger |0\rangle = d_1^\dagger \ldots d_n^\dagger |\psi\rangle \qquad (2b.24)$$

for all $n \geq 0$. The unitarity of W implies that $d_k^\dagger$ satisfy the CAR and hence that $\mathcal{W}$ is an isometry. It is also clear that $\mathcal{W}$ satisfies (2b.12).

To show that $\mathcal{W}$ is unitary we first observe that $|0\rangle$ can be written as a linear combination of vectors of the form (2b.24). This is easily seen by interchanging the roles of $|0\rangle$ and $|\psi\rangle$ and of W and $W^\dagger$ in the argument which led to the construction, (2b.13), of $|\psi\rangle$. From this it follows that all simple vectors $c_1^\dagger \ldots c_n^\dagger|0\rangle$ can be written as combinations of the vectors of the form (2b.24). Indeed, from (2b.14), $c_k^\dagger = c^\dagger((uu^\dagger + vv^\dagger)f_k) + c((u\overline{v}^\dagger + v\overline{u}^\dagger)\overline{f}_k) = d^\dagger(u^\dagger f_k) + d(\overline{v}^\dagger \overline{f}_k)$. Thus $\mathcal{W}$ is invertible and hence unitary. ■

2.3 THEOREM: *Let $0 \leq \Gamma \leq \mathbf{1}$ be an operator on $\mathcal{H} \oplus \mathcal{H}$ of the form (2b.5), subject to (2b.8), and assume furthermore that* $\mathrm{Tr}[\gamma] < \infty$. *Then there exists a unique quasi-free state ρ with finite particle number such that Γ is the 1-pdm of ρ.*

Remark: Suppose we are given a γ satisfying $0 \leq \gamma \leq 1$. We can set $\Gamma = \begin{pmatrix} \gamma & 0 \\ 0 & 1-\gamma \end{pmatrix}$, i.e. set $\alpha = 0$ and, according to Theorem 2.3, we can extend Γ to a quasi-free state ρ. In other words, given γ we can find a **particle conserving** quasi-free state having this γ as its 1-*pdm* (whether or not $\mathrm{Tr}\gamma$ is an integer). By a **particle conserving state** we mean a state (such as a Gibbs state for a particle conserving Hamiltonian) that is a convex combination of states, each having a definite particle number, i.e. there are no cc or $c^\dagger c^\dagger$ matrix elements in this state, which is the same thing as saying $\alpha = 0$. However, unless γ is a projection (i.e., a usual HF state) Γ cannot have a *definite* particle number, i.e. $\rho(\mathcal{N}^2) > \rho(\mathcal{N})^2$. In fact, defining $\rho(\mathcal{N}^2) = \sum_N N^2 \rho(\pi^{(N)}) = \sum_{k,l} \rho(c_k^\dagger c_k c_l^\dagger c_l)$, we can use (2a.12) to compute

$$\rho(\mathcal{N}^2) = \rho(\mathcal{N})^2 + \sum_{k,l}\left(\gamma_{lk}\gamma_{kl} + \alpha_{lk}^\dagger \alpha_{lk}\right) + \sum_k \gamma_{kk} = \rho(\mathcal{N})^2 + \mathrm{Tr}[\gamma - \gamma^2] + \mathrm{Tr}[\alpha^\dagger \alpha], \qquad (2b.25)$$

from which we see that $\rho(\mathcal{N}^2) = \rho(\mathcal{N})^2$ requires *both* $\alpha = 0$ *and* $\gamma^2 = \gamma$.

Proof: Since $\mathrm{Tr}[\gamma]$ is finite it is clear from the form in (2b.5) that although $\mathrm{Tr}[\Gamma]$ may be infinite, which is the case when $\dim \mathcal{H} = \infty$, we have $\mathrm{Tr}[\Gamma(\mathbf{1} - \Gamma)] < \infty$. Thus, there is an orthonormal basis of eigenvectors for $\Gamma(\mathbf{1} - \Gamma)$. If φ is an eigenvector for $\Gamma(\mathbf{1} - \Gamma)$ of eigenvalue μ then so is $\Gamma\varphi$ and, since $\Gamma^2\varphi = \Gamma\varphi - \mu\varphi$, it follows that Γ leaves invariant the subspace space $\{\varphi, \Gamma\varphi\}$, which is at most 2-dimensional. We conclude that there is an orthonormal basis of eigenvectors for Γ.

If $\varphi = f \oplus g$ is a normalized eigenvector for Γ of eigenvalue λ then, by (2b.5) and (2b.8), we find that $\widetilde{\varphi} = \overline{g} \oplus \overline{f}$ is a normalized eigenvector for Γ of eigenvalue $(1 - \lambda)$. Thus, we can find a unitary W on $\mathcal{H}\oplus\mathcal{H}$ of the form (2a.9) such that (using the basis $f_1, f_2, \ldots$ for both copies of $\mathcal{H}$) the four blocks of the transformed Γ have the form

$$W^\dagger \Gamma W = \begin{pmatrix} \lambda_1 & & & & & \\ & \lambda_2 & & & 0 & \\ & & \ddots & & & \\ & & & 1-\lambda_1 & & \\ & 0 & & & 1-\lambda_2 & \\ & & & & & \ddots \end{pmatrix}, \tag{2b.26}$$

with $0 \le \lambda_i \le 1/2$ for $i = 1, 2, \ldots$. Using this and $\mathrm{Tr}[\Gamma(\mathbf{1}-\Gamma)] < \infty$, we obtain $\sum_i \lambda_i < \infty$.

We shall now prove that W satisfies the condition of Theorem 2.2, i.e., that $\mathrm{Tr}[vv^\dagger] < \infty$ and hence that W corresponds to a Bogoliubov transformation $\mathcal{W}$ on $\mathcal{F}$. Indeed, from (2b.26) we know that the upper left block of the matrix $W^\dagger \Gamma W$ has finite trace, i.e.,

$$\mathrm{Tr}[u^\dagger \gamma u + \overline{v}^\dagger \alpha^\dagger u + u^\dagger \alpha \overline{v} + \overline{v}^\dagger (1-\overline{\gamma})\overline{v}] < \infty. \tag{2b.27}$$

Since $0 \le \Gamma \le \mathbf{1}$ we have that $\Gamma^2 \le \Gamma$. The upper left block of this inequality reads $\gamma^2 + \alpha\alpha^\dagger \le \gamma$. Thus $\mathrm{Tr}[\alpha\alpha^\dagger] \le \mathrm{Tr}[\gamma] < \infty$. By Cauchy-Schwarz we estimate

$$\begin{aligned} \mathrm{Tr}[u^\dagger \gamma u + \overline{v}^\dagger \alpha^\dagger u + &u^\dagger \alpha \overline{v} + \overline{v}^\dagger (1-\overline{\gamma})\overline{v}] - \mathrm{Tr}[\overline{v}^\dagger \overline{v}] \\ &= \mathrm{Tr}[u^\dagger \gamma u + \overline{v}^\dagger \alpha^\dagger u + u^\dagger \alpha \overline{v} - \overline{v}^\dagger \overline{\gamma v}] \\ &\ge -\mathrm{Tr}[uu^\dagger \gamma] - 2\mathrm{Tr}[\overline{v}^\dagger \overline{v}]^{1/2} \mathrm{Tr}[uu^\dagger \alpha\alpha^\dagger]^{1/2} - \mathrm{Tr}[\overline{v}\,\overline{v}^\dagger \overline{\gamma}] \\ &\ge -2\mathrm{Tr}[\gamma] - 2\mathrm{Tr}[\overline{v}^\dagger \overline{v}]^{1/2} \mathrm{Tr}[\gamma]^{1/2}. \end{aligned} \tag{2b.28}$$

We conclude from (2.31) that $\mathrm{Tr}[\overline{v}^\dagger \overline{v}] - 2\mathrm{Tr}[\overline{v}^\dagger \overline{v}]^{1/2}\mathrm{Tr}[\gamma]^{1/2} < \infty$ and hence that $\mathrm{Tr}[vv^\dagger] = \mathrm{Tr}[\overline{v}^\dagger \overline{v}] < \infty$.

If we prove that the diagonal matrix $W^\dagger \Gamma W$ is the 1-*pdm* of a quasi-free state $\widetilde{\rho}$ then we know that Γ is the 1-*pdm* of the state ρ with $\rho(A) = \widetilde{\rho}(\mathcal{W}^\dagger A \mathcal{W})$. We may therefore assume that Γ is itself diagonal of the form (2.26).

Let Π_0 be the projection onto the subspace of $\mathcal{F}$ on which $\sum_{i:\lambda_i=0} c_i^\dagger c_i = 0$.

For each i such that $\lambda_i > 0$ choose e_i to satisfy

$$(1+\exp(e_i))^{-1} = \lambda_i, \tag{2b.29}$$

(note that $0 \le e_i < \infty$, since $0 < \lambda_i \le 1/2$) and consider the following (possibly unbounded) operator H on $\mathcal{F}$.

$$H = \sum_{i:\lambda_i \ne 0} e_i c_i^\dagger c_i. \tag{2b.30}$$

We shall now prove that the operator

$$G := \Pi_0 \exp(-H) \tag{2b.31}$$

has finite trace on $\mathcal{F}$ and that the state

$$\rho(A) = \mathrm{Tr}[G]^{-1}\mathrm{Tr}[AG] \tag{2b.32}$$

is quasi-free and has Γ as its 1-*pdm*. It is easy to see that the trace of G is

$$\mathrm{Tr}[G] = \prod_{i:\lambda_i\neq 0}[1+\exp(-e_i)] = \prod_i (1-\lambda_i)^{-1} < \infty, \tag{2b.33}$$

since $\sum_i \lambda_i < \infty$.

The operator G looks peculiar but, by introducing the operator $H' = \sum_{i:\lambda_i=0} c_i^\dagger c_i$ which commutes with H, we can write the state ρ as a limit of Gibbs states:

$$\rho(A) = \lim_{\beta\to\infty} Z_\beta^{-1}\mathrm{Tr}[A\exp(-\beta H' - H)]. \tag{2b.34}$$

It is well-known (see [GM] for a simple proof) that the Gibbs state for an operator of the form $\sum_i e_i c_i^\dagger c_i$ is quasi-free. Hence we conclude (by taking the limit $\beta\to\infty$) that ρ is quasi-free.

The fact that Γ is the 1-*pdm* of ρ follows from the computation

$$\begin{aligned}\rho((c_k^\dagger + c_l)(c_m + c_n^\dagger)) &= \mathrm{Tr}[G]^{-1}\mathrm{Tr}[(c_k^\dagger + c_l)(c_m + c_n^\dagger)G] \\ &= \delta_{km}\mathrm{Tr}[G]^{-1}\mathrm{Tr}[c_k^\dagger c_k G] + \delta_{ln}\mathrm{Tr}[G]^{-1}\mathrm{Tr}[c_l c_l^\dagger G] \\ &= \prod_i(1-\lambda_i)\left(\delta_{km}\lambda_k(1-\lambda_k)^{-1}\prod_{i:i\neq k}(1-\lambda_i)^{-1} + \delta_{ln}\prod_{i:i\neq l}(1-\lambda_i)^{-1}\right) \\ &= \delta_{km}\lambda_k + \delta_{ln}(1-\lambda_l), \end{aligned} \tag{2b.35}$$

where we have used the fact that $\exp[-e_k] = \lambda_k(1-\lambda_k)^{-1}$ if $\lambda_k\neq 0$. Finally ρ has finite particle number since $\rho(\mathcal{N}) = \mathrm{Tr}[\gamma]$.

The uniqueness of ρ follows as in the remark after (2b.8): The 1-*pdm* of a quasi-free state determines the state. ∎

We call an operator Γ **admissible** if it satisfies the properties in Theorem 2.3, i.e., is of the form (2b.5) subject to (2b.8) with $\mathrm{Tr}[\gamma]<\infty$ and $0\leq\Gamma\leq\mathbf{1}$. We then have that:

Γ *is admissible if and only if it is the 1-pdm of a generalized Hartree-Fock state.*

In the above proof we not only proved the existence of a quasi-free state having Γ as its 1-*pdm*, we also gave the explicit form of ρ. To make this more explicit we introduce the following notion:

Quadratic Hamiltonian: *A self-adjoint operator H (bounded or unbounded) on $\mathcal{F}$ is said to be a quadratic Hamiltonian if the unitary operators $\mathcal{W}(t) := \exp(iHt)$ are Bogoliubov transformations for all t.*

If H is a quadratic Hamiltonian there correspond operators $W(t)$ on $\mathcal{H}\oplus\mathcal{H}$ of the form (2a.9) corresponding to the Bogoliubov transformations $\mathcal{W}(t)$. Since the anticommutator satisfies

$$\left\{c^\dagger(\overline{h}_2) + c(h_1), \exp(iHt)\left(c^\dagger(g_1) + c(\overline{g}_2)\right)\exp(-iHt)\right\} = \left\langle \begin{pmatrix} h_1 \\ h_2\end{pmatrix} \,\middle|\, W(t)\begin{pmatrix} g_1 \\ g_2\end{pmatrix}\right\rangle \mathbf{1}, \tag{2b.36}$$

it follows that $W(t)$ is a strongly continuous one-parameter group of unitaries on $\mathcal{H}\oplus\mathcal{H}$. Hence there is a self-adjoint operator A (bounded or unbounded) such that $W(t) = \exp(iAt)$.

The operator A has the block structure

$$A = \begin{pmatrix} a & b \\ b^\dagger & -\overline{a} \end{pmatrix}, \tag{2b.37}$$

where a and b are operators on $\mathcal{H}$ with $a^\dagger = a$ and $b^T = -b$.

We call[†] the operator A the **first quantization of** H and we call H *a* **second quantization of** A. Notice that from (2b.36) A is determined uniquely by H. If H is a bounded operator on $\mathcal{F}$ then A is bounded on $\mathcal{H} \oplus \mathcal{H}$ and by differentiating (2b.36) we can, in this case, write

$$\{c^\dagger(\overline{h}_2) + c(h_1), [H, c^\dagger(g_1) + c(\overline{g}_2)]\} = \left\langle \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \middle| A \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \right\rangle \mathbf{1}. \tag{2b.38}$$

Here we have introduced the commutator $[K_1, K_2] := K_1K_2 - K_2K_1$.

The operator H , however, is only determined by A up to addition of a multiple of the identity. If A is bounded we may write the *unique* second quantization, H, of A satisfying $\langle 0|H|0\rangle = 0$ in terms of the matrix elements of a and b, as

$$H = \sum_{i,j} a_{ij} c_i^\dagger c_j + \tfrac{1}{2} \sum_{i,j} \left(b_{ij} c_i^\dagger c_j^\dagger + b_{ij}^\dagger c_i c_j \right). \tag{2b.39}$$

If H is a quadratic Hamiltonian and if $\mathcal{W}$ is a Bogoliubov transformation then $\mathcal{W}H\mathcal{W}^\dagger$ is also a quadratic Hamiltonian. If H is a second quantization of A then $\mathcal{W}H\mathcal{W}^\dagger$ is a second quantization of $WAW^\dagger$, where W is the unitary given in (2a.9).

The proof of Theorem 2.3 implies the following result about the structure of quasi-free states.

2.4 LEMMA: *Let ρ be a quasi-free state with finite particle number, i.e., $\rho(\mathcal{N}) < \infty$ (in terms of its 1-pdm this means $\mathrm{Tr}[\gamma] < \infty$). Then there exist two commuting quadratic Hamiltonians H and H' (possibly $H = 0$ or $H' = 0$, but not both) such that*

$$\rho(B) = \lim_{\beta\to\infty} \mathrm{Tr}[\exp(-\beta H' - H)]^{-1} \mathrm{Tr}[B \exp(-\beta H' - H)]. \tag{2b.40}$$

This means that the state ρ is a product of the ground state (zero temperature state) for H' and the Gibbs state for H. Thus if $H' = 0$, ρ is a Gibbs state and if $H = 0$, ρ is a pure state. In the next two lemmas we discuss quasi-free Gibbs states and quasi-free pure states in more detail.

2.5 LEMMA: *If A is an operator on $\mathcal{H} \oplus \mathcal{H}$ of the form (2b.37) then*

$$\Gamma := (\mathbf{1} + \exp(A))^{-1} \tag{2b.41}$$

is of the form (2b.5) subject to (2b.8). Furthermore, if this Γ satisfies $\mathrm{Tr}[\gamma] < \infty$, so that it defines a quasi-free state ρ by Theorem 2.3, then this ρ is given by

$$\rho(B) = \mathrm{Tr}[\exp(-H)]^{-1} \mathrm{Tr}[B \exp(-H)], \tag{2b.42}$$

where H is any second quantization of A.

[†] Our terminology is far from being conventional, but it is descriptive.

Conversely, if ρ in (2b.42) is a quasi-free state of finite particle number with 1-pdm Γ, then H is quadratic with first quantization satisfying (2b.41).

Proof: Let U be the unitary

$$U = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \tag{2b.43}$$

on $\mathcal{H} \oplus \mathcal{H}$. Then $UAU^\dagger = -\overline{A}$, since A has the form (2b.37). Hence, $U\Gamma U^\dagger = \mathbf{1} - \overline{\Gamma}$ which proves that Γ is of the form (2b.5) subject to (2b.8).

If Γ satisfies $\mathrm{Tr}[\gamma] < \infty$ it follows from the proof of Theorem 2.3 that there is a Bogoliubov transformation $\mathcal{W}$ with corresponding W such that the $W^\dagger \Gamma W$, which is the 1-*pdm* of the transformed state $\rho_{\mathcal{W}}$, is diagonal in our chosen basis. We denote by $\lambda_1, \lambda_2, \ldots$, those eigenvalues of $W^\dagger \Gamma W$ in the interval $[0, 1/2)$ together with half the eigenvalues equal to $1/2$ (if any). The other half of the eigenvalues of $W^\dagger \Gamma W$ are then given by $1 - \lambda_1, 1 - \lambda_2, \ldots$. The operator $W^\dagger A W$ is also diagonal with the first half of the eigenvalues given by $e_1, e_2, \ldots$ and the second half by $-e_1, -e_2, \ldots$, according to the definition (2b.41).

Since

$$\exp\Big(i\sum_k e_k c_k^\dagger c_k\Big) c_l^\dagger \exp\Big(-i\sum_k e_k c_k^\dagger c_k\Big) = \exp(ie_l) c_l^\dagger \tag{2b.44}$$

we see that the second quantizations of $W^\dagger A W$ are of the form $\widetilde{H}_\tau = \sum_k e_k c_k^\dagger c_k + \tau \mathbf{1}$, where τ is any real number. Since the Gibbs states are independent of τ we see that all the operators $\widetilde{H}_\tau$ define the same Gibbs state as the operator in (2.33), i.e., the state $\rho_{\mathcal{W}}$. (As in (2b.42) we are referring to Gibbs states with the inverse temperature $\beta = 1$.)

Since $\rho_{\mathcal{W}}$ is the Gibbs state for $\widetilde{H}_\tau$, the state ρ is given by

$$\rho(B) = \rho_{\mathcal{W}}(\mathcal{W}^\dagger B \mathcal{W}) = \mathrm{Tr}[\exp(-\widetilde{H}_\tau)]^{-1} \mathrm{Tr}[\mathcal{W}^\dagger B \mathcal{W} \exp(-\widetilde{H}_\tau)], \tag{2b.45}$$

which agrees with (2b.42) if $H = \mathcal{W}\widetilde{H}_\tau \mathcal{W}^\dagger$. Such an H is however, a second quantization of $WW^\dagger AWW^\dagger = A$.

The converse statement is also a simple consequence of the proof of Theorem 2.3. One only has to realize that the state ρ in (2b.42) uniquely determines the operator H. ■

2.6 THEOREM: *A quasi free state ρ with finite particle number is a pure state $\rho(B) = \langle\psi|B|\psi\rangle$ if and only if the 1-pdm Γ with $\mathrm{Tr}[\gamma] < \infty$ is a projection on $\mathcal{H} \oplus \mathcal{H}$, i.e., $\Gamma^2 = \Gamma$.*

In terms of Γ the vector $|\psi\rangle$ is of the form (2b.13) but this time with $g_1, \ldots, g_r, h_1, k_1, \ldots$ being orthonormal eigenvectors of γ; the vectors $g_1, \ldots g_r$ with eigenvalue 1 and the pair $h_1, k_i := -(\zeta_i - \zeta_i^2)^{-1/2} \alpha \overline{h_i}$ with eigenvalue ζ_i, where $0 < \zeta_i < 1$.

Proof: Let ρ be a pure state. Since ρ is uniquely determined by its 1-*pdm* Γ, we may assume it to be of the form (2b.32). The purity of ρ, then, is equivalent to G being rank one and hence $\lambda_i = 0$ for all i, which is equivalent to Γ to be a projection.

Again from the proof of Theorem 2.3 the diagonal form of Γ is

$$W^\dagger \Gamma W = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1} \end{pmatrix}. \tag{2b.46}$$

Hence

$$\Gamma = W \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1} \end{pmatrix} W^\dagger = \begin{pmatrix} vv^\dagger & v\overline{u}^\dagger \\ \overline{u}v^\dagger & \overline{u}\,\overline{u}^\dagger \end{pmatrix} \tag{2b.47}$$

and we have $\gamma = vv^\dagger$ and $\alpha = v\overline{u}^\dagger = -u\overline{v}^\dagger$. Since $W^\dagger \Gamma W$ is the 1-*pdm* of the pure state corresponding to the vacuum, Γ is the 1-*pdm* of the pure state corresponding to $|\psi\rangle = \mathcal{W}|0\rangle$. Here $\mathcal{W}$ is the Bogoliubov transform defined by W. The last statement of the lemma now follows by comparison with Theorem 2.2. ■

Using this lemma we can find a basis for $\mathcal{H}\oplus\mathcal{H}$ where the blocks γ and α of Γ take a particularly simple form when Γ is a projection. In fact, if we choose the basis consisting of $g_i \oplus 0, l_i \oplus 0, h_i \oplus k_i$ and $0 \oplus \overline{g}_i, 0 \oplus \overline{l}_i, \overline{k}_i \oplus \overline{h}_i$ for all $i = 1, 2, \ldots$, we find (with $\alpha_i = (\zeta_i - \zeta_i^2)^{-1/2}$)

$$\gamma = \begin{pmatrix} \ddots & & & \\ & \zeta_i & & \\ & & \zeta_i & \\ & & & \ddots \end{pmatrix} \quad \text{and} \quad \alpha = \begin{pmatrix} \ddots & & & \\ & 0 & \alpha_i & \\ & -\alpha_i & 0 & \\ & & & \ddots \end{pmatrix}. \tag{2b.48}$$

2.7 LEMMA: *Let ρ be a pure and quasi-free state of finite particle number with 1-pdm Γ. Then $\rho(\mathcal{N}^2) < \infty$ and it is given by (2b.49) with α given in (2b.5).*

$$\rho(\mathcal{N}^2) - \rho(\mathcal{N})^2 = 2\mathrm{Tr}[\alpha^\dagger \alpha]. \tag{2b.49}$$

This equation shows that ρ is not necessarily a fixed particle number state.

Proof: Since ρ is pure, Γ is a projection and hence $\gamma = \gamma^2 + \alpha\alpha^\dagger$ which together with (2b.25) implies (2b.49).■

From Lemma 2.7 we see that a generalized HF state with 1-*pdm* Γ has conserved particle number if and only if the component α of Γ vanishes. We call a generalized HF state for which this holds a **normal state**.

II.c THE GENERALIZED HF FUNCTIONAL

In this section we shall introduce the generalized Hartree-Fock approximation for a self-adjoint operator H on Fock space of the form

$$H = \widehat{h} + \widehat{V}, \tag{2c.1}$$

where $\widehat{h}$ is a quadratic (particle number preserving) operator

$$\widehat{h} = \sum_{i,j} h_{ij} c_i^\dagger c_j, \tag{2c.2}$$

and $\widehat{V}$ is a **quartic operator** (again particle number preserving)

$$\widehat{V} = \tfrac{1}{2} \sum_{k,l,m,n} V_{kl;mn} c_k^\dagger c_l^\dagger c_n c_m. \tag{2c.3}$$

By (2c.2) the operator $\widehat{h}$ is defined in terms of matrix elements h_{ij} of a self-adjoint operator h on $\mathcal{H}$. The operator h is the restriction of $\widehat{h}$ to the one-body space $\mathcal{H}^{(1)} = \mathcal{H}$, i.e.,

$$h_{ij} = \langle f_i | h | f_j \rangle = \langle 0 | c_i \widehat{h} c_j^\dagger | 0 \rangle. \tag{2c.4}$$

By (2c.3) the operator $\widehat{V}$ is defined in terms of matrix elements $V_{kl;mn}$ of a self-adjoint operator V on $\mathcal{H}\otimes\mathcal{H}$. Note that we are not restricting V to be an operator on the antisymmetric two-body space $\mathcal{H}^{(2)} = \mathcal{H} \wedge \mathcal{H}$. The restriction of V to the antisymmetric subspace is equal to the restriction of $\widehat{V}$ to $\mathcal{H}^{(2)}$.

$$\begin{aligned}\langle 0|c_l c_k \widehat{V} c_m^\dagger c_n^\dagger|0\rangle &= \tfrac{1}{2}(V_{kl;mn} + V_{lk;nm} - V_{kl;nm} - V_{lk;mn}) \\ &= \tfrac{1}{2}\langle f_k \wedge f_l|V|f_m \wedge f_n\rangle. \end{aligned} \tag{2c.5}$$

The operators V and h defining $\widehat{V}$ and $\widehat{h}$ may be bounded or unbounded. We shall, however, assume that the operator H is bounded below This is the case if, for example, $\widehat{h}$ and $\widehat{V}$ are bounded below. One way to ensure this is to assume that h and V are bounded below by (negative) operators of finite trace (it is not enough to assume that h and V are bounded below in order to have $\widehat{h}$ and $\widehat{V}$ bounded below.).

The expressions (2c.2–3) are somewhat formal. A more precise definition can be given as follows. On each $\mathcal{H}^{(N)}$ we can, in the obvious way, define the sum $h^{(N)} = \sum_{i=1}^N h_i$ of N commuting copies of h and the corresponding sum $V^{(N)} = \sum_{1\le i<j\le N} V_{ij}$ of N commuting copies of V. Then $H = \sum_N (h^{(N)} + V^{(N)})\Pi^{(N)}$.

In discussing Hamiltonians of the form (2c.1) we have two particular examples in mind. The first is the *Hubbard Hamiltonian* defined in Sect. III. The second is the *atomic Hamiltonian* with $\mathcal{H}$ being the square integrable (spinor valued) functions on $\mathbf{R}^3$ and $h = -(\hbar^2/2m)\Delta - Z/|x| - \mu$, where $\mu \le 0$ is a chemical potential and $V = e^2|x-y|^{-1}$. Both h and V are independent of (diagonal in) spin. The Hubbard Hamiltonian is a bounded operator (in fact a finite dimensional matrix) while the atomic Hamiltonian is unbounded but bounded below. [If $\mu < 0$ then h and V are bounded below by operators of finite trace, but if $\mu = 0$, h will not be bounded below by such an operator (e.g., the negative eigenvalues of hydrogen are not summable). This, however, is not a real problem because the operator H is still bounded below.]

For both the Hubbard Hamiltonian and the atomic Hamiltonian we shall be interested in the ground state and its energy. The ground state is simply the (maybe not unique) state ρ_0 (with finite particle number) for which $\rho(H)$ takes on the smallest possible value – the ground state energy – provided this smallest value is attained for some state at all. Otherwise the ground state does not exist.

If H is unbounded the expectation $\rho(H)$ is not necessarily well-defined. If, however, H is bounded below we can define $\rho(H)$. This is easy to see for states that can be written as $\rho(B) = \mathrm{Tr}[GB]$ for some positive operator G of finite trace on Fock space (this is not true for all states, but we are only interested in states for which it holds). If H is bounded from below, we can without loss of generality assume that H is positive. Then $\mathrm{Tr}[GH]$ is, when expanded in the eigenvector basis for G, an infinite sum of positive terms. This sum then defines $\rho(H)$ (possibly to be $+\infty$).

The expected number of particles in the ground state is $\rho(\mathcal{N})$. Since both Hamiltonians are particle number preserving there is a ground state ρ with a fixed number of particles, i.e., $\rho(\mathcal{N}^2) = \rho(\mathcal{N})^2$. The number of particles $N := \rho(\mathcal{N})$ is thus an integer and ρ is, in fact, a state on $\mathcal{H}^{(N)}$ (i.e., $\rho(\Pi^{(N)}) = 1$).

Alternatively to specifying a chemical potential μ, we could also have specified the number N and then considered the problem on $\mathcal{H}^{(N)}$. The equivalence of the two descriptions by Legendre transform (equivalence of the grand canonical and canonical ensembles) requires that the ground state energy is a convex function of the particle number. While this is believed to be the case there is, to the best of our knowledge, no rigorous proof of this fact in the two models discussed. In the grand canonical picture the ground state energy *is* a concave function of the chemical potential, but as long as we do not know the convexity of the canonical energy as a function of N we cannot assert that the two energy functions are Legendre transforms of each other. Here we shall mostly work in the grand canonical framework, i.e., specify a chemical potential, except at the end of the section where we shall discuss the canonical picture when V is assumed to be positive.

In addition to the ground state energy we shall also be interested in the grand canonical Gibbs states $\rho(B) = Z^{-1}\mathrm{Tr}[B\exp(-\beta H)]$. The Gibbs state, however, is not well defined for the atomic Hamiltonian since the operator $\exp(-\beta H)$ will not have finite trace in this case.

The object of study in this section is not the real ground states and Gibbs states but rather their (generalized) Hartree-Fock approximations which we shall now define.

The Hartree-Fock approximation to the ground state is simply the generalized Hartree-Fock state with least possible energy. By Theorem 2.3 there is a one-to-one correspondence between a generalized HF state ρ and its 1-*pdm* Γ. We may therefore define the **generalized Hartree-Fock energy functional**,

$$\mathcal{E}(\Gamma) = \rho(H), \tag{2c.6}$$

on the set of all admissible density matrices.

The energy of a generalized Hartree-Fock state can be computed in terms of the 1-*pdm* Γ as follows. The expectation of the quadratic part is $\rho(\widehat{h}) = \mathrm{Tr}[h\gamma]$. In computing the expectation of the quartic part we apply (2.12) and obtain

$$\rho(\widehat{V}) = \tfrac{1}{2}\sum_{k,l,m,n} V_{kl;mn}\left(\gamma_{mk}\gamma_{nl} - \gamma_{ml}\gamma_{nk} + \alpha^{\dagger}_{lk}\alpha_{mn}\right). \tag{2c.7}$$

The operator $G^{(2)}$ on $\mathcal{H}\otimes\mathcal{H}$ with matrix elements $G^{(2)}_{mn;kl} = \gamma_{mk}\gamma_{nl} - \gamma_{ml}\gamma_{nk} + \alpha^{\dagger}_{lk}\alpha_{mn}$ has finite trace. In fact, if we choose $V = I$ in (2c.7) we obtain $\widehat{V} = \mathcal{N}(\mathcal{N}-1)$ and $\mathrm{Tr}[G^{(2)}] = \rho(\mathcal{N}^2) - \rho(\mathcal{N})$ which is finite by Lemma 2.7.

Equation (2c.7) states that $\rho(\widehat{V}) = \frac{1}{2}\mathrm{Tr}[VG^{(2)}]$. Both $\mathrm{Tr}[VG^{(2)}]$ and $\mathrm{Tr}[h\gamma]$ are well-defined since V and h are bounded from below and $G^{(2)}$ and γ are positive operators of finite trace.

As mentioned after (2a.12) the three terms in (2b.9) are called respectivley the **direct energy**, the **exchange energy** and the **pairing energy**.

We can thus write the HF energy functional as

$$\mathcal{E}(\Gamma) = \mathrm{Tr}[h\gamma] + \tfrac{1}{2}\sum_{k,l,m,n} V_{kl;mn}\left(\gamma_{mk}\gamma_{nl} - \gamma_{ml}\gamma_{nk} + \alpha^{\dagger}_{lk}\alpha_{mn}\right). \tag{2c.8}$$

The **Hartree-Fock energy** is given by

$$E^{\mathrm{HF}} := \inf\left\{\mathcal{E}(\Gamma) \mid \Gamma \text{ is an admissible density matrix}\right\}. \tag{2c.9}$$

As we have proved the one-to-one correspondence between quasi-free states and admissible density matrices, (2c.9) is evidently equivalent to

$$E^{\mathrm{HF}} := \inf\left\{\rho(H) \mid \rho \text{ is a quasi-free state}\right\}. \tag{2c.10}$$

We shall not discuss, in general, whether the infimum in (2c.9) is attained. For the Hubbard Hamiltonian, however, it is clearly the case that the infimum in (2c.9) is attained since the set of admissible denisity matrices is a compact subset of a finite dimensional space. In case of the *atomic Hamiltonian* it is also true that the infimum is attained. This result was proved in [LS], where it was assumed that $\alpha = 0$, but this follows from Theorem 2.11 below). A 1-*pdm* for which the infimum (2c.9) is attained defines a **HF ground state**.

To define the finite temperature **HF Gibbs state** we must introduce the **entropy of a quasi-free state**:

$$S(\Gamma) := -\tfrac{1}{2}\mathrm{Tr}[\Gamma \ln \Gamma] - \tfrac{1}{2}\mathrm{Tr}[(\mathbf{1}-\Gamma)\ln(\mathbf{1}-\Gamma)] = -\mathrm{Tr}[\Gamma \ln \Gamma]. \tag{2c.10}$$

The last equality in (2c.10) holds because Γ and $\mathbf{1} - \overline{\Gamma}$ are unitarily equivalent (cf. proof of Lemma 2.5) and Γ has real eigenvalues. Notice that by Theorem 2.6, $S(\Gamma) = 0$ if and only if Γ is the 1-*pdm* of a pure state.

We define the **Hartree-Fock pressure functional** $\mathcal{P}_\beta$ at inverse temperature β as

$$-\mathcal{P}_\beta(\Gamma) = \mathcal{E}(\Gamma) - \beta^{-1}S(\Gamma). \tag{2c.11}$$

The **Hartree-Fock pressure** is defined by

$$\mathcal{P}^{\mathrm{HF}}(\beta) = \sup\left\{\mathcal{P}_\beta(\Gamma) \mid \Gamma \text{ is an admissible density matrix}\right\}. \tag{2c.12}$$

As explained above we only consider positive temperature in case of the Hubbard Hamiltonian and as for the energy it is then clear that the supremum is attained. A HF Gibbs state is defined by a 1-*pdm* maximizing (2c.11).

In the next lemma we show that the HF energy gives an upper bound to the true energy and the HF pressure gives a lower bound to the true pressure.

2.8 THEOREM: *We have the inequality*

$$E^{\mathrm{HF}} \geq E^{\mathrm{Q}} := \inf_\rho \rho(H), \tag{2c.13}$$

where the infimum is over all states ρ (not just HF states). If $\widehat{h}$ and $\widehat{V}$ are bounded

$$\mathcal{P}^{\mathrm{HF}}(\beta) \leq \mathcal{P}^{\mathrm{Q}} := \beta^{-1}\ln \mathrm{Tr}[\exp(-\beta H)]. \tag{2c.14}$$

Proof: The inequality (2c.13) is obvious since E^{HF} is defined according to (2c.10) as an infimum over a restricted class of states, namely the generalized HF states.

Inequality (2c.14) is more complicated. The aim is to show that for any generalized HF state ρ with 1-*pdm* Γ we have

$$\exp(-\beta\rho(H) + S(\Gamma)) \leq \mathrm{Tr}[\exp(-\beta H)]. \tag{2c.15}$$

According to Lemma 2.4 any generalized HF state is a limit (in the sense of convergence of expectation values of bounded operators) of quasi-free Gibbs states. Moreover, it is clear that the entropies of the approximating Gibbs states are greater than the entropy of the limiting state. We can therefore assume that the quasi-free state ρ in (2c.15) is a Gibbs state.

Since ρ is a Gibbs state we can define an operator A on $\mathcal{H} \oplus \mathcal{H}$ as in (2b.41). This operator is then the first quantization of a quadratic operator h_A and

$$\rho(B) = \mathrm{Tr}[\exp(-\beta h_A)]^{-1}\mathrm{Tr}[B\exp(-\beta h_A)]. \tag{2c.16}$$

To specify h_A uniquely we assume that $\langle 0|h_A|0\rangle = 0$.

By the Peierls-Bogoliubov inequality [TW] we infer

$$\begin{aligned}\mathrm{Tr}[\exp(-\beta H)] =& \mathrm{Tr}[\exp(-\beta(h_A + H - h_A)] \\ \geq& \mathrm{Tr}[\exp(-\beta h_A)] \exp(-\beta\rho(H - h_A)).\end{aligned} \tag{2c.17}$$

The inequality (2c.14) follows if we can prove

$$S(\Gamma) = \beta\rho(h_A) + \ln\Big(\mathrm{Tr}[\exp(-\beta h_A)]\Big). \tag{2c.18}$$

By diagonalizing the operator A as in the proof of Lemma 2.5 we find

$$\mathrm{Tr}[\exp(-\beta h_A)] = \prod_k (1 + \exp(-\beta e_k)), \tag{2c.19}$$

where $e_1, e_2, \dots$ again denote the positive eigenvalues of A and half the zero eigenvalues (if any). We also find

$$\rho(h_A) = \mathrm{Tr}[\exp(-\beta h_A)]^{-1}\mathrm{Tr}[h_A \exp(-\beta h_A)] = \sum_k e_k[1 + \exp(\beta e_k)]^{-1}. \tag{2c.20}$$

Using (2b.41), (2c.19) and (2c.20) we finally obtain that the right side of (2c.18) is

$$\sum_k \ln\Big(1 + \exp(\beta e_k)\Big) + \sum_k \beta e_k \left(\Big(1 + \exp(\beta e_k)\Big)^{-1} - 1\right) = \tfrac{1}{2}\mathrm{Tr}\Big[-\ln(\Gamma) - (\mathbf{1} - \Gamma)\ln(\Gamma^{-1} - \mathbf{1})\Big], \tag{2c.21}$$

which is exactly $S(\Gamma)$. ■

It is always possible to choose the quantum ground state to be a pure state. The same is true in generalized HF theory. This follows from the next lemma when compared with Theorem 2.6.

2.9 THEOREM: *The infimum of $\mathcal{E}$ over all admissible density matrices agrees with the infimum over all admissible projections, i.e.,*

$$E^{\mathrm{HF}} = \inf\{\mathcal{E}(\Gamma) \mid \Gamma \textit{ is admissible and } \Gamma^2 = \Gamma\}. \tag{2c.22}$$

Proof: We shall show that for any admissible Γ there is a projection Γ_0 such that $\mathcal{E}(\Gamma_0) \leq \mathcal{E}(\Gamma)$. For this purpose it suffices to approximate h and V by bounded operators — for which there is obviously no difficulty with convergence of the following sums.

For any admissible Γ, as in the proof of Theorem 2.3, we can find a Bogoliubov transformation $\mathcal{W}$ with corresponding W such that $W^\dagger\Gamma W$ is diagonal. If Γ is the 1-*pdm* of the state ρ then $W^\dagger\Gamma W$ is the 1-*pdm* of the transformed state $\rho_{\mathcal{W}}$. We have the relation $\mathcal{E}(\Gamma) = \rho(H) = \rho_{\mathcal{W}}(\mathcal{W}^\dagger H\mathcal{W})$. The transformed Hamiltonian $\mathcal{W}^\dagger H\mathcal{W}$ is also a sum of a quadratic operator $\mathcal{W}^\dagger\widehat{h}\mathcal{W}$ and a quartic operator $\mathcal{W}^\dagger\widehat{V}\mathcal{W}$, but these are not necessarily number preserving. If we (anti)commute all $c^\dagger$ to the left (normal ordering) we obtain

$$\mathcal{W}^\dagger H\mathcal{W} = \sum_{i,j}\widetilde{h}_{ij}c_i^\dagger c_j + \tfrac{1}{2}\sum_{kl;mn}\widetilde{V}_{kl;mn}c_k^\dagger c_l^\dagger c_n c_m + \kappa\mathbf{1} + R, \tag{2c.23}$$

where $\widetilde{h}_{ij}$ and $\widetilde{V}_{kl;mn}$ are new matrix elements and κ is some constant. The operator R contains all particle non-conserving terms of the form

$$cc, \quad c^\dagger c^\dagger, \quad cccc, \quad c^\dagger ccc, \quad c^\dagger c^\dagger c^\dagger c, \quad c^\dagger c^\dagger c^\dagger c^\dagger. \tag{2c.24}$$

Since $\rho_{\mathcal{W}}(R) = 0$, we obtain

$$\mathcal{E}(\Gamma) = \rho_{\mathcal{W}}(\mathcal{W}^\dagger H \mathcal{W}) = \kappa + \sum_i \widetilde{h}_{ii}\lambda_i + \tfrac{1}{2}\sum_{kl}(\widetilde{V}_{kl;kl} - \widetilde{V}_{kl;lk})\lambda_k\lambda_l, \tag{2c.25}$$

where $\lambda_1, \lambda_2, \ldots,$ are as usual the eigenvalues of Γ smaller than 1/2.

The important fact to observe about the expression in (2c.25) is that, although it is a quadratic form in $\lambda_1, \lambda_2, \ldots$, it is linear in each variable. Hence $\partial\mathcal{E}(\Gamma)/\partial\lambda_j$ is independent of λ_j. Therefore, we do not increase the energy expectation by replacing $\lambda_j|\varphi_j\rangle\langle\varphi_j| + (1-\lambda_j)|U\overline{\varphi}_j\rangle\langle U\overline{\varphi}_j|$ in Γ by $|\varphi_j\rangle\langle\varphi_j|$ in case $\partial\mathcal{E}(\Gamma)/\partial\lambda_j < 0$ and by $|U\overline{\varphi}_j\rangle\langle U\overline{\varphi}_j|$ otherwise. Proceeding this way, we arrive at a 1-*pdm* Γ_0 with energy no greater than before and with all eigenvalues either 0 or 1. This means that Γ_0 is a projection. ■

If ρ is a generalized HF ground state for H we define a corresponding **HF mean field Hamiltonian**. It is the following quadratic Hamiltonian written in terms of the blocks γ and α of the 1-*pdm* Γ of ρ.

$$H_\rho := \sum_{i,j} h_{ij} c_i^\dagger c_j + \tfrac{1}{2}\sum_{kl;mn} V_{kl;mn}\Big[\gamma_{km}c_l^\dagger c_n + \gamma_{nl}c_k^\dagger c_m - \gamma_{ml}c_k^\dagger c_n - \gamma_{nk}c_l^\dagger c_m + \alpha_{lk}^\dagger c_n c_m + \alpha_{mn}c_k^\dagger c_l^\dagger\Big]. \tag{2c.26}$$

A HF ground state of H is **self-consistent** in the sense given in the next lemma.

2.10 LEMMA: *If ρ is a HF ground state for the Hamiltonian H, i.e., a HF minimizer, then ρ is a true (not just HF) ground state for the Hamiltonian H_ρ.*

Proof: We must show that $\rho(H_\rho) \le \rho'(H_\rho)$ for any state ρ' with finite particle number.

From the 1-*pdm* Γ' of ρ' and the 1-*pdm* Γ of ρ we can for $0 \le t \le 1$ construct a new 1-*pdm* $\Gamma_t = (1-t)\Gamma + t\Gamma'$. Then Γ_t is admissible and since Γ is a minimizer for $\mathcal{E}$ we have

$$0 \le \frac{d\mathcal{E}(\rho_t)}{dt}\Big|_{t=0} = \rho'(H_\rho) - \rho(H_\rho), \tag{2c.27}$$

which proves the claim. It is important here that since H_ρ is quadratic, $\rho'(H_\rho)$ depends only on the 1-*pdm* of ρ'. ■

Although, we can always find a state with fixed particle number among the quantum ground states for the Hamiltonian H, this may not be the case for the generalized HF ground states, as discussed in the introduction (and proved for the attractive Hubbard Hamiltonian in Sect. III). Here there need not be a normal ground state.

It is often stated in the literature that if the HF ground state is not a normal state, (i.e., it is a BCS state) the potential V must have a negative component. It is now very easy to state this precisely.

2.11 THEOREM: *If the operator V is positive (semi) definite on $\mathcal{H}\otimes\mathcal{H}$*

$$E^{\mathrm{HF}} = \inf\{\mathcal{E}(\Gamma) \mid \Gamma \textit{ is admissible and normal, i.e., } \alpha = 0\}. \tag{2c.28}$$

Moreover, if V is strictly positive (i.e., positive definite) then any ground state (if it exists) must be a normal state. Likewise, we have for the pressure

$$\mathcal{P}^{\mathrm{HF}}(\beta) = \sup\{\mathcal{P}_\beta(\Gamma) \mid \Gamma \textit{ is admissible and normal }\}. \tag{2c.29}$$

Proof: That V is positive means that for all $g \in \mathcal{H}\otimes\mathcal{H}$ we have

$$\sum_{kl;mn} V_{kl;mn}\overline{g}_{kl}g_{mn} \geq 0. \tag{2c.30}$$

Strict positivity means that if $g \neq 0$ then (2.67) is a strict inequality. The pairing energy is exactly of the form (2.67) hence

$$\sum_{kl;mn} V_{kl;mn}\alpha^\dagger_{lk}\alpha_{mn} = \sum_{kl;mn} V_{kl;mn}\overline{\alpha}_{kl}\alpha_{mn} \geq 0. \tag{2c.31}$$

Assume Γ is admissible with non-zero α and form a new operator $\widetilde{\Gamma}$ by replacing α by zero. It is clear that $\widetilde{\Gamma}$ is still admissible and by (2c.31) that $\mathcal{E}(\widetilde{\Gamma})$ is (strictly) smaller than $\mathcal{E}(\Gamma)$ if V is (strictly) positive. To prove the result on the pressure we notice that the 1-*pdm* Γ' obtained by changing α to $-\alpha$ is unitarily equivalent to Γ. Hence, since the entropy is a concave function we find

$$S(\widetilde{\Gamma}) = S(\tfrac{1}{2}\Gamma + \tfrac{1}{2}\Gamma') \geq \tfrac{1}{2}S(\Gamma) + \tfrac{1}{2}S(\Gamma') = S(\Gamma). \tag{2c.32}$$

■

In the remainder of this section we shall specialize to the case of positive V and discuss the canonical picture. Thus, instead of a chemical potential we now fix the value $\mathrm{Tr}[\gamma] = N$. Since we have $\alpha = 0$ it is enough to consider the component γ of Γ.

The discussion is of special interest in the atomic case where the potential V *is* strictly positive.

There is a version of Theorem 2.9 for the canonical case of fixed particle number N. We state it below without proof. It is, in fact, more difficult to prove than Theorem 2.9 because in deforming γ to a projection we have to keep $\mathrm{Tr}[\gamma] = N$. The proof was first given in [LE1] (see [BV] for a simple proof).

2.12 THEOREM (Variational principle): *If V is positive then*

$$\begin{aligned} E^{\mathrm{HF}}(N) :&= \inf\{\mathcal{E}(\gamma) \mid \gamma \textit{ is admissible with } \mathrm{Tr}[\gamma] = N\} \\ &= \inf\{\mathcal{E}(\gamma) \mid \gamma \textit{ is an admissible projection with } \mathrm{Tr}[\gamma] = N]\}. \end{aligned} \tag{2c.33}$$

Moreover, if V is strictly positive then any HF minimizer must be a projection.

Combining Theorem 2.11 and Theorem 2.12 we see that a HF ground state ρ for a system with strictly positive V is not only particle conserving ($\alpha = 0$) but, in fact, has fixed particle number, i.e., $\rho(\mathcal{N}^2) = \rho(\mathcal{N})^2$.

Theorem 2.12 is useful in many cases for obtaining upper bounds to the Hartree-Fock energy, E^{HF}, and hence an upper bound to the true quantum energy, E^Q. It allows one to deal conveniently with what is sometimes called the "orthogonality problem". Take any matrix γ satisfying $0 \leq \gamma \leq \mathbf{1}$ (as an operator) and $\mathrm{Tr}\gamma = N$, and compute the one-body energy

$$E_1(\gamma) = \mathrm{Tr}\gamma h = \sum_{i,j} \gamma_{ij} h_{ji} \tag{2c.34}$$

and the two body energy

$$E_2(\gamma) = \tfrac{1}{2} \sum_{k,l,m,n} V_{kl;mn}(\gamma_{mk}\gamma_{nl} - \gamma_{ml}\gamma_{nk}) \tag{2c.35}$$

Then

$$E^Q \leq E^{\mathrm{HF}} \leq E_1(\gamma) + E_2(\gamma). \tag{2c.36}$$

The important point here is that the matrix $\gamma_{mk}\gamma_{nl} - \gamma_{ml}\gamma_{nk}$ is not, in general, the two-body reduced density matrix of *any* N-body density matrix *unless* γ comes from a Slater determinant, i.e., $\gamma_{ij} = \sum_{\alpha=1}^{N} \varphi_i^\alpha \overline{\varphi}_j^\alpha$, with $\varphi^1, \ldots, \varphi^N$ being N orthonormal functions. Nevertheless, (2c.36) continues to be true.

Contrary to the proof of Theorem 2.9 the proof of Lemma 2.10 is unchanged in the canonical case (because the 1-*pdm* $\gamma_t = (1-t)\gamma + t\gamma'$, automatically satisfies $\mathrm{Tr}[\gamma_t] = N$ if $\mathrm{Tr}[\gamma] = N$ and $\mathrm{Tr}[\gamma'] = N$).

2.13 LEMMA: *If V is positive and if ρ is a HF ground state for the Hamiltonian H under the constraint $\rho(\mathcal{N}) = N$ then ρ is a true ground state for the Hamiltonian H_ρ under the same constraint.*

The mean field Hamiltonian has a simpler form when restricted to fixed particle number.

$$H_\rho := \sum_{i,j} h_{ij} c_i^\dagger c_j + \tfrac{1}{2} \sum_{kl;mn} V_{kl;mn} \Big[\gamma_{km} c_l^\dagger c_n + \gamma_{nl} c_k^\dagger c_m - \gamma_{ml} c_k^\dagger c_n - \gamma_{nk} c_l^\dagger c_m \Big], \tag{2c.37}$$

which is simply a (number preserving) independent particle Hamiltonian.

When V is strictly positive we can prove a much stronger result than Lemma 2.13. Namely, not only is a HF ground state, ρ, for H a true ground state for the mean field operator H_ρ, but it is the *unique* ground state for H_ρ satisfying the constraint $\rho(\mathcal{N}) = N$.

This uniqueness result is equivalent to the striking statement made in the introduction, that *no degenerate energy levels of H_ρ (if they exist) can be only partially filled in the HF state.* We empasize again how contradictory this is to what is taught in elementary chemistry courses. We learn in the theory of chemical binding how two unpaired electrons in separate atoms can pair up and create a strongly bound molecule. The concept of unpaired electrons relies of course essentially on the independent orbital picture of HF theory. What we prove is that there are *no unpaired* electrons in HF theory.

The obvious question is of course: *But what then has happened to the spin degeneracy?* The answer is, as already discussed, that there may not be spin degeneracy in HF theory, because even the spin symmetry can be broken. Likewise for the angular momentum degeneracy; there may not be spherical symmetry.

The following is the theorem that there are no unfilled shells. It was proved by M. Loss and the authors [BLL]. Since the proof is very short we repeat it here.

2.14 THEOREM: (Shells are always closed.) *Assume that the two-body potential V in the Hamiltonian H is strictly positive (as in Coulomb case). If ρ is a HF ground state (a Slater determinant state) for H, i.e., a HF minimizer subject to the constraint $\rho(\mathcal{N}) = N$, then ρ is the unique ground state of the mean field operator H_ρ satisfying the constraint $\rho(\mathcal{N}) = N$.*

Proof: From Theorem 2.12 we know that the 1-*pdm* γ of ρ is an N-dimensional projection, which we can write

$$\gamma = \sum_{j=1}^{N} |g_j\rangle\langle g_j|, \tag{2c.38}$$

where $g_1, g_2, \ldots$ are N orthonormal eigenvectors of γ. Since ρ is a ground state for H_ρ we can assume that $g_1, g_2, \ldots$ are eigenvectors of H_ρ.

If there is another ground state with the same number of electrons there must be a degenerate level containing a vector from γ, say g_N, and at the same time a normalized eigenvector g' which is not in γ, i.e., with $\gamma g' = 0$. We can then define a new N-dimensional projection by

$$\gamma' = |g'\rangle\langle g'| + \sum_{j=1}^{N-1} |g_j\rangle\langle g_j|. \tag{2c.39}$$

The HF state ρ' with 1-*pdm* γ' is then also a ground state for H_ρ, i.e., $\rho(H_\rho) = \rho'(H_\rho)$.

Since γ is a minimizer for the HF functional we have

$$\begin{aligned} 0 \leq &\mathcal{E}(\gamma') - \mathcal{E}(\gamma) - (\rho'(H_\rho) - \rho(H_\rho)) \\ =&\tfrac{1}{2} \sum_{kl;mn} V_{kl;mn} \Big[(\gamma-\gamma')_{mk}(\gamma-\gamma')_{nl} - (\gamma-\gamma')_{nk}(\gamma-\gamma')_{ml} \Big]. \end{aligned} \tag{2c.40}$$

The operator $\gamma - \gamma' = |g_N\rangle\langle g_N| - |g'\rangle\langle g'|$. Hence, since V is strictly positive,

$$\begin{aligned} \tfrac{1}{2} \sum_{kl;mn} & V_{kl;mn} \Big[(\gamma-\gamma')_{mk}(\gamma-\gamma')_{nl} - (\gamma-\gamma')_{nk}(\gamma-\gamma')_{ml} \Big] \\ =&\langle g_N \otimes g_N | V | g_N \otimes g_N\rangle + \langle g' \otimes g' | V | g' \otimes g'\rangle - \langle g_N \otimes g' | V | g_N \otimes g'\rangle \\ &- \langle g' \otimes g_N | V | g' \otimes g_N\rangle - \langle g_N \otimes g_N | V | g_N \otimes g_N\rangle - \langle g' \otimes g' | V | g' \otimes g'\rangle \\ &+ \langle g_N \otimes g' | V | g' \otimes g_N\rangle + \langle g' \otimes g_N | V | g_N \otimes g'\rangle \\ =&\langle g_N \wedge g' | V | g' \wedge g_N\rangle < 0, \end{aligned} \tag{2c.41}$$

which contradicts (2c.40). ■

To illustrate this result let us consider the simple, but not altogether trivial example of $N = 1$ for the atomic Hamiltonian. In this case the HF ground state energy is in fact the true ground state energy. It is simply the ground state energy of hydrogen (with nuclear charge Z), i.e, $-\frac{1}{4}Z^2$ in our units. Owing to the spin degeneracy the ground state is doubly degenerate. We consider the spin up ground state and write it $\psi = |\varphi(x)\uparrow\rangle$. Here we have used the hydrogen ground state wave function $\varphi(x) = CZ^{3/2}\exp(-Z|x|)$. It is important to realize that the mean field operator corresponding to ψ is not just the hydrogen operator, but rather the operator H_ψ that acts on a general $\psi' = |\varphi'(x)\sigma\rangle$, with $\sigma =\uparrow$ or $\sigma =\downarrow$ according to

$$\begin{aligned} H_\psi|\varphi'(x)\sigma\rangle = &\left(-\Delta - \frac{Z}{|x|} + \int \varphi(y)^2|x-y|^{-1}dy\right)|\varphi'(x)\sigma\rangle \\ &- \delta_{\sigma\uparrow}\int \varphi(y)\varphi'(y)|x-y|^{-1}dy|\varphi'(x)\sigma\rangle. \end{aligned} \tag{2c.42}$$

Notice that H_ψ is spin dependent — it does not commute with spin rotations.

The mean field operator and the hydrogen operator agree on their common ground state ψ, i.e.,

$$H_\psi\psi = \left(-\Delta - \frac{Z}{|x|}\right)\psi = -\tfrac{1}{4}Z^2\psi. \tag{2c.43}$$

On the other ground state for hydrogen, namely, $|\varphi\downarrow\rangle$ we find, however,

$$\begin{aligned} \langle\varphi\downarrow|H_\psi|\varphi\downarrow\rangle = &\langle\varphi\downarrow|\left(-\Delta - \frac{Z}{|x|}\right)|\varphi\downarrow\rangle + \iint \varphi(x)^2\varphi(y)^2|x-y|^{-1}dxdy \\ = &-\tfrac{1}{4}Z^2 + cZ. \end{aligned} \tag{2c.44}$$

Thus the mean field operator induces a gap in the energy between the two degenerate ground states of hydrogen.

Theorem 2.14 states that this is not only true for the state $|\varphi\downarrow\rangle$, but in fact, the ground state for H_ψ is *unique*. More importantly, by Theorem 2.14 this is not particular to the case $N = 1$.

III. THE GENERALIZED HF THEORY FOR THE HUBBARD MODEL WITH ATTRACTIVE INTERACTION

III.a DEFINITIONS

In this section the generalized HF theory will be applied to the Hubbard model with attractive interaction. Our *main result* (Theorem 3.12) in Sect. III.e) will be that the HF ground state and positive temperature Gibbs state are unique, modulo global gauge transformations. First, we recall the definition of the Hubbard model. Let Λ be a finite lattice, i.e., a finite collection of points, and let $|\Lambda|$ be the number of these points. The one-particle Hilbert space $\mathcal{H}$ is the $2|\Lambda|$-dimensional space of spinor-valued functions on Λ, i.e., the set of complex-valued functions on $\Lambda \times \{-1,1\}$. The value of such a function at (y,τ) (with $y \in \Lambda, \tau \in \{-1,1\}$) is $f(y,\tau)$ and the inner product is $\langle f|g\rangle = \sum_{y,\tau}\overline{f}(y,\tau)g(y,\tau)$. A canonical orthonormal basis in $\mathcal{H}$ is given by the delta functions, which we denote by $|x,\sigma\rangle$. Thus, $|x,\sigma\rangle \in \mathcal{H}$ is the function $f_{x,\sigma}(y,\tau) = \delta_{y,x}\delta_{\tau,\sigma}$. We define our complex conjugation in this basis. In the Fock space $\mathcal{F}$ corresponding to $\mathcal{H}$ we refer to $c^\dagger(|x,\sigma\rangle)$ as $c^\dagger_{x,\sigma}$. We often use the abbreviation $\uparrow := +1$ and $\downarrow := -1$. An orthonormal basis in $\mathcal{F}$ is given by $\{c^\dagger_{x_1,\sigma_1}\ldots c^\dagger_{x_N,\sigma_N}|0\rangle \mid (x_i,\sigma_i) \neq (x_j,\sigma_j) \text{ if } i \neq j\}$, which implies that $\mathcal{F}$ is $4^{|\Lambda|}$-dimensional.

The Hubbard Hamiltonian for negative coupling is

$$H_- = \sum_{\substack{x,y\in\lambda \\ \sigma}} t_{xy}c^\dagger_{x,\sigma}c_{y,\sigma} - \sum_{x\in i} U_x\left(c^\dagger_{x,\uparrow}c_{x,\uparrow} - \tfrac{1}{2}\right)\left(c^\dagger_{x,\downarrow}c_{x,\downarrow} - \tfrac{1}{2}\right). \tag{3a.1}$$

The second term in H_- is an attractive interaction among the electrons with position dependent coupling $-U_x < 0$. (Our notation here and elsewhere is that $U_x \geq 0$.) Other authors frequently replace the last two factors in (3a.1) by $(c^\dagger_{x\uparrow}c_{x\uparrow})(c^\dagger_{x\downarrow}c_{x\downarrow})$, but we prefer our form (also used in [LLM]) because it preserves hole-particle symmetry; if U_x is independent of x the distinction is unimportant. In the first term, the $|\Lambda| \times |\Lambda|$ self-adjoint matrix $t = \{t_{xy}\}_{x,y\in\Lambda}$ is called the **hopping matrix**. Since we shall later include a chemical potential we can and will assume without loss of generality that $\mathrm{Tr}[t] = 0$. We do not assume $t_{xx} = 0$, but when t is bipartite (defined below) the condition $t_{xx} = 0$ is automatic. We emphasize that up to this point Λ was an arbitrary set and need not have any topological structure. It is the structure of t, linking different points in Λ, that makes the embedding of Λ into $\mathbf{R}^d$ sometimes useful. Indeed, in the original model introduced by Hubbard, Kanamori and Gutzwiller [HJ], [KJ], [GMC], Λ is a finite cube of lattice points in $\mathbf{Z}^d$ and $t_{xy} := \tau$ when x and y are nearest neighbors, and $t_{xy} = 0$ otherwise. The imposition of periodic boundary conditions makes Λ into a d-dimensional discrete torus on which t is translation invariant. Let us remark that, except in Sect. III.g, we shall neither assume that t is translation invariant nor that U_x is constant. However, connectedness, reality and bipartiteness of t will play an important role in our analysis. These notions can be conveniently characterized by means of path. A **path** is an ordered sequence $\{x_1, x_2, \ldots, x_n\}$ of points in Λ such that $t_{x_1x_2}, t_{x_2x_3}, \ldots, t_{x_{n-1}x_n}$ are all non-vanishing. We will always assume t to be **connected**, i.e., any two points $x, y \in \Lambda$ are linked by a path $\{x, x_1, \ldots, x_n, y\}$. We say t is **real** if $t_{xy} \in \mathbf{R}$ for all $x, y \in \Lambda$. For real t self-adjointness implies that $t_{xy} = \bar{t}_{yx} = t_{yx}$. For every closed path $\{x_1, x_2, \ldots, x_n, x_1\}$ the product $t_{x_1x_2}t_{x_2x_3}\ldots t_{x_nx_1}$ obviously yields a real number provided t is real. Conversely, if $t_{x_1x_2}\ldots t_{x_nx_1}$ is real for every closed path then t is unitarily equivalent to some real hopping matrix $t' = WtW^\dagger$ where W is a gauge transformation (see [LL] Lemma 2.1). Hence, unless there is at least one closed path for which $t_{x_1x_2}\ldots t_{x_nx_1}$ is not real, we may as well assume that t is real.

The matrix t is said to be **bipartite** if there are two disjoint subsets $A, B \subseteq \Lambda$ with $A \cup B = \Lambda$, such that $t_{xy} = 0$ whenever both $x, y \in A$ or $x, y \in B$. Evidently, t is bipartite if and only if all paths contain an even number of points.

One important property of a bipartite t is that it is unitarily equivalent to $-t$. Indeed, defining the unitary $|\Lambda| \times |\Lambda|$-matrix $(-1)^x = [(-1)^x]^{-1} = [(-1)^x]^\dagger$ by

$$(-1)^x := \sum_{x\in A} |x\rangle\langle x| - \sum_{x\in B} |x\rangle\langle x|, \tag{3a.2}$$

one easily checks that

$$(-1)^x t (-1)^x = -t. \tag{3a.3}$$

If it is unambigously clear from the context what is meant, we will use the same symbol $(-1)^x$ to denote the function which takes the value 1 on the A sublattice and -1 on the B sublattice. The Dirac notation is used in (3a.2), whereby $|\varphi\rangle\langle\varphi|$ denotes the projection onto a normalized vector φ. The vector x is here the delta function $\delta_{x,\cdot}$ at $x \in \Lambda$ in the space of complex-valued functions $\mathcal{H}_\Lambda$ on Λ (not $\Lambda \times \{\uparrow, \downarrow\}$). Let us now make a few remarks about the different Hilbert spaces we will encounter in what follows. We start with $\mathcal{H}_\Lambda$. Mathematically we may view the one-particle Hilbert space $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{H}_\Lambda \oplus \mathcal{H}_\Lambda = \mathbf{C}^2 \otimes \mathcal{H}_\Lambda \tag{3a.4}$$

and, consequently, the space on which the 1-*pdm* are defined as

$$\mathcal{H} \oplus \mathcal{H} = \mathbf{C}^4 \otimes \mathcal{H}_\Lambda. \tag{3a.5}$$

(We wrote equalities in (3a.4) and (3a.5) despite of our awareness that an isomorphism would have been mathematically more appropriate.) It is thus clear that operators on $\mathcal{H} = \mathcal{H}_\Lambda \oplus \mathcal{H}_\Lambda$ can be written as 2×2-matrices with operators on $\mathcal{H}_\Lambda$ as entries and, likewise, operators on $\mathcal{H} \oplus \mathcal{H}$ as 4×4-matrices with operators on $\mathcal{H}_\Lambda$ as entries. The usual conventions for matrix algebras are understood and, in particular,

$$q \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} := \begin{pmatrix} qm_{11} & qm_{12} \\ qm_{21} & qm_{22} \end{pmatrix}, \tag{3a.6}$$

where q and m_{ij} are complex numbers or operators on $\mathcal{H}_\Lambda$, and likewise for 4×4-matrices. It will often be convenient for us to change between the Hilbert spaces $\mathcal{H}_\Lambda$, $\mathcal{H}$, and $\mathcal{H} \oplus \mathcal{H}$, and to take traces over these various spaces. To simplify notations we shall use a common symbol, Tr, for these traces; the Hilbert space in question will be evident from the operator whose trace is being computed. Likewise, we shall denote the identity operator on these different spaces be the common symbol $\mathbf{1}$. It will always be clear from the context which identity we are refering to.

We are now in a position to write down the pressure functional for the Hubbard model. We choose to define the 1-*pdm* in terms of the orthonormal basis of delta functions $|x, \sigma\rangle$. Hence, the energy expectation for a 1-*pdm* $0 \le \Gamma = \begin{pmatrix} \gamma & \alpha \\ \alpha^\dagger & \mathbf{1} - \overline{\gamma} \end{pmatrix} \le \mathbf{1}$ is given by

$$\begin{aligned} \mathcal{E}(\Gamma) = \mathrm{Tr}[t\gamma] - \sum_{x \in \Lambda} U_x \big\{ & [\langle x \uparrow |\gamma| x \uparrow\rangle - \tfrac{1}{2}][\langle x \downarrow |\gamma| x \downarrow\rangle - \tfrac{1}{2}] \\ & - |\langle x, \uparrow |\gamma| x, \downarrow\rangle|^2 + |\langle x \uparrow |\alpha| x \downarrow\rangle|^2 \big\}. \end{aligned} \tag{3a.7}$$

Here, we identified t with the operator $\begin{pmatrix} t & 0 \\ 0 & t \end{pmatrix}$ on $\mathcal{H}$.

The thermodynamic pressure of Γ (actually, the pressure multiplied by the "volume") is given by (with $\beta = 1/k_{\mathrm{Boltzmann}} T$)

$$\begin{aligned} -\mathcal{P}_{\beta,\mu}(\Gamma) &= \mathcal{E}(\Gamma) - \beta^{-1} S(\Gamma) - \mu N(\Gamma) \\ &= \mathcal{E}(\Gamma) + \tfrac{1}{2}\beta^{-1} \mathrm{Tr}[\Gamma \ln \Gamma + (\mathbf{1} - \Gamma) \ln(\mathbf{1} - \Gamma)] - \mu \mathrm{Tr}[\gamma]. \end{aligned} \tag{3a.8}$$

We have here introduced the chemical potential μ. We could equivalently have replaced the Hamiltonian H_- by $H_- - \mu \mathcal{N}$, where $\mathcal{N}$ is the particle number operator. Also we have introduced the notation $N(\Gamma) := \mathrm{Tr}[\gamma]$ for the particle number expectation in the state described by Γ.

Our aim is to characterize the set of maximizing 1-*pdm*'s for the pressure (which we typically denote by Γ_0) as explicitly as possible and to determine the pressure $\mathcal{P}(\beta, \mu)$ of the system, i.e.,

$$\mathcal{P}(\beta, \mu) := \max\{\mathcal{P}_{\beta,\mu}(\Gamma) \mid 0 \le \Gamma = \begin{pmatrix} \gamma & \alpha \\ \alpha^\dagger & \mathbf{1} - \overline{\gamma} \end{pmatrix} \le \mathbf{1}\} = \mathcal{P}_{\beta,\mu}(\Gamma_0). \tag{3a.9}$$

A priori, the *max* in (3a.9) should be replaced by *supremum* but, since the underlying Hilbert space is finite dimensional, the existence of at least one maximizing 1-*pdm* is assured.

III.b LINEARIZATION OF THE PRESSURE FUNCTIONAL

As a first illustration of the notation introduced above, a 1-*pdm* Γ as an operator on $\mathbf{C}^4 \otimes \mathcal{H}_\Lambda$, is written as

$$\Gamma = \begin{pmatrix} \gamma_\uparrow & \gamma_* & \alpha_\uparrow & \alpha_* \\ \gamma_*^\dagger & \gamma_\downarrow & -\alpha_*^T & \alpha_\downarrow \\ \alpha_\uparrow^\dagger & -\overline{\alpha_*} & \mathbf{1} - \overline{\gamma_\uparrow} & \overline{\gamma_*} \\ \alpha_*^\dagger & \alpha_\downarrow^\dagger & \overline{\gamma}_*^\dagger & \mathbf{1} - \overline{\gamma_\downarrow} \end{pmatrix}, \tag{3b.1}$$

where $\langle x|\gamma_\sigma|y\rangle := \langle x,\sigma|\gamma|y,\sigma\rangle$, $\langle x|\gamma_*|y\rangle := \langle x,\uparrow|\gamma|y,\downarrow\rangle$, $\langle x|\alpha_\sigma|y\rangle := \langle x,\sigma|\alpha|y,\sigma\rangle$, and $\langle x|\alpha_*|y\rangle := \langle x,\uparrow|\alpha|y,\downarrow\rangle$. Now, observe that $\mathcal{E}(\Gamma)$ depends neither on $\alpha_\uparrow$ nor on $\alpha_\downarrow$, and that $\mathcal{E}(\Gamma)$ would be lowered, if we were allowed to replace γ_* by 0. Indeed, as the following lemma shows, a restriction of our attention to the 1-*pdm* with $\alpha_\uparrow, \alpha_\downarrow$ and γ_* all equal to zero and, moreover, $\gamma_\uparrow = \gamma_\downarrow$ and $\alpha_* = \alpha_*^T$ is justified. Such matrices are of the form (with empty spaces denoting zeros)

$$\Gamma = \begin{pmatrix} \gamma' & & & \alpha' \\ & \gamma' & -\alpha' & \\ & -\alpha'^\dagger & \mathbf{1} - \overline{\gamma'} & \\ \alpha'^\dagger & & & \mathbf{1} - \overline{\gamma'} \end{pmatrix}, \tag{3b.2}$$

where $\gamma' = \gamma'^\dagger$ and $\alpha'^T = \alpha'$.

3.1 LEMMA: For all $\beta > 0$ (including the $\beta = \infty$) and all μ we have

$$-\mathcal{P}(\beta,\mu) = \min\{-\mathcal{P}_{\beta,\mu}(\Gamma) \mid \Gamma \text{ of the form (3b.2) and satisfying } 0 \le \Gamma \le \mathbf{1}\}.$$

Proof: Define two orthogonal projections on $\mathcal{H} \oplus \mathcal{H}$ by

$$P := \begin{pmatrix} 0 & & & \\ & \mathbf{1} & & \\ & & \mathbf{1} & \\ & & & 0 \end{pmatrix}, \qquad \widetilde{P} := \begin{pmatrix} \mathbf{1} & & & \\ & 0 & & \\ & & 0 & \\ & & & \mathbf{1} \end{pmatrix}. \tag{3b.3}$$

Clearly, $P\widetilde{P} = 0$ and $P + \widetilde{P} = \mathbf{1}$. Observe that for any 1-*pdm* Γ written as in (3b.1), we have

$$\widetilde{\Gamma} := P\Gamma P + \widetilde{P}\Gamma\widetilde{P} = \begin{pmatrix} \gamma_\uparrow & & & \alpha_* \\ & \gamma_\downarrow & -\alpha_* & \\ & -\alpha_*^\dagger & \mathbf{1} - \overline{\gamma}_\uparrow & \\ \alpha_*^\dagger & & & \mathbf{1} - \overline{\gamma}_\downarrow \end{pmatrix}. \tag{3b.4}$$

This operator $\widetilde{\Gamma}$ is also of the desired form (3b.1). Moreover, $0 \le \widetilde{\Gamma} = P\Gamma P + \widetilde{P}\Gamma\widetilde{P} \le P + \widetilde{P} = \mathbf{1}$ and hence $\widetilde{\Gamma}$ is a 1-*pdm*. As remarked above, $\mathcal{E}(\widetilde{\Gamma}) \le \mathcal{E}(\Gamma)$ and $N(\widetilde{\Gamma}) = N(\Gamma)$. It remains to show that $-S(\widetilde{\Gamma}) \le -S(\Gamma)$. We recall that $A \mapsto \mathrm{Tr}\{f(A)\}$ is a concave function of the self-adjoint operator A if $f : \mathbf{R} \to \mathbf{R}$ is concave, i.e., $f(\lambda x + (1-\lambda)y) \ge \lambda f(x) + (1-\lambda) f(y)$ for all x, y and all $0 \le \lambda \le 1$. Applying this to $f(x) := x \ln x + (1-x)\ln(1-x)$, we observe that $S(\Gamma)$ is concave in Γ;

$$S(\tfrac{1}{2}\Gamma_1 + \tfrac{1}{2}\Gamma_2) \ge \tfrac{1}{2}S(\Gamma_1) + \tfrac{1}{2}S(\Gamma_2), \tag{3b.5}$$

for all 1-*pdm* Γ_1 and Γ_2. We evaluate (3b.5) on $\Gamma_1 := \Gamma$ and $\Gamma_2 := (P - \widetilde{P})\Gamma(P - \widetilde{P})$, the latter being a 1-*pdm* since $P - \widetilde{P}$ is unitary and preserves the form (3b.1). But, using the unitarity of $P - \widetilde{P}$ again, (3b.5) yields

$$S(\widetilde{\Gamma}) = S(\tfrac{1}{2}\Gamma_1 + \tfrac{1}{2}\Gamma_2) \ge \tfrac{1}{2}S(\Gamma) + \tfrac{1}{2}S((P-\widetilde{P})\Gamma(P-\widetilde{P})) = S(\Gamma). \tag{3b.6}$$

Hence, we may restrict the variation to 1-*pdm* $\widetilde{\Gamma}$ of the form (3b.4).

Moreover, defining the unitary

$$W = \begin{pmatrix} 0 & \mathbf{1} & & \\ -\mathbf{1} & 0 & & \\ & & 0 & \mathbf{1} \\ & & -\mathbf{1} & 0 \end{pmatrix}, \tag{3b.7}$$

we observe that $W\widetilde{\Gamma}W^\dagger$ coincides with $\widetilde{\Gamma}$ except that $\gamma_\uparrow$ and $\gamma_\downarrow$ are interchanged as are α_* and α_*^T. Hence,

$$\widehat{\Gamma} := \tfrac{1}{2}\widetilde{\Gamma} + \tfrac{1}{2}W\widetilde{\Gamma}W^\dagger = \begin{pmatrix} \gamma' & & & \alpha' \\ & \gamma' & -\alpha' & \\ & -\alpha'^\dagger & \mathbf{1}-\overline{\gamma'} & \\ \alpha'^\dagger & & & \mathbf{1}-\overline{\gamma'} \end{pmatrix}, \tag{3b.8}$$

where $\gamma' := \frac{1}{2}(\gamma_\uparrow + \gamma_\downarrow)$ and $\alpha' := \frac{1}{2}(\alpha_* + \alpha_*^T)$.

As before, concavity of S implies

$$S(\widehat{\Gamma}) = S(\tfrac{1}{2}\widetilde{\Gamma} + \tfrac{1}{2}W\widetilde{\Gamma}W^\dagger) \ge \tfrac{1}{2}S(\widetilde{\Gamma}) + \tfrac{1}{2}S(W\widetilde{\Gamma}W^\dagger) = S(\Gamma), \tag{3b.9}$$

with equality if and only if $\widehat{\Gamma} = \widetilde{\Gamma}$. We have $N(\Gamma) = N(\widehat{\Gamma})$ and

$$\begin{aligned} \mathcal{E}(\Gamma) - \mathcal{E}(\widehat{\Gamma}) = \sum_x U_x \big\{ & \tfrac{1}{4}[\langle x|\gamma_\uparrow|x\rangle + \langle x|\gamma_\downarrow|x\rangle - 1]^2 \\ & - [\langle x|\gamma_\uparrow|x\rangle - \tfrac{1}{2}][\langle x|\gamma_\downarrow|x\rangle - \tfrac{1}{2}]\big\} \ge 0 \end{aligned} \tag{3b.10}$$

with equality if and only if $\langle x|\gamma_\uparrow|x\rangle = \langle x|\gamma_\downarrow|x\rangle$ for all $x \in \Lambda$. ■

Thanks to Lemma 3.1 we may now restrict ourselves to 1-*pdm* of the form (3b.2) for which the 4×4-matrix formalism is clearly redundant. Indeed, introducing the unitary operator

$$Y := \begin{pmatrix} \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} \\ 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & -\mathbf{1} & 0 \end{pmatrix} \tag{3b.11}$$

on $\mathcal{H} \oplus \mathcal{H}$, one easily checks that Γ in (3b.2) becomes

$$Y\Gamma Y^\dagger = \begin{pmatrix} \gamma' & \alpha' & & \\ \alpha'^\dagger & \mathbf{1}-\overline{\gamma}' & & \\ & & \gamma' & \alpha' \\ & & \alpha'^\dagger & \mathbf{1}-\overline{\gamma}' \end{pmatrix} =: \begin{pmatrix} \Gamma' & \\ & \Gamma' \end{pmatrix}. \tag{3b.12}$$

Although it seems that the conditions that Γ be a 1-*pdm* on $\mathcal{H}\oplus\mathcal{H}$ are equivalent to the conditions for Γ' to be a 1-*pdm* on $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$, there is one important difference. We must require Γ' to satisfy $0\le\Gamma'\le\mathbf{1}$ and to be of the form

$$\Gamma' = \begin{pmatrix} \gamma' & \alpha' \\ \alpha'^\dagger & \mathbf{1}-\overline{\gamma}' \end{pmatrix}, \tag{3b.13}$$

with

$$(\gamma')^\dagger = \gamma', \qquad \alpha'^T = \alpha'. \tag{3b.14}$$

Because of this difference we will distinguish between $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$ and $\mathcal{H}$, even though they are isomorphic. Physically, $\mathcal{H}$ is the space of spin-up and spin-down particles whereas the action of Y shows that $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$, on which Γ' is defined, is rather the space of spin-up particles and spin-down holes.

We shall denote the projection operator in $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$ which projects onto (functions non-vanishing only at) the site $x\in\Lambda$ by $\mathbf{1}_x$. The diagonal part of a 1-*pdm* Γ' is denoted by

$$\Gamma'_x := \mathbf{1}_x\Gamma'\mathbf{1}_x = \begin{pmatrix} \gamma'(x) & \alpha'(x) \\ \overline{\alpha}'(x) & \mathbf{1}-\gamma'(x) \end{pmatrix}\mathbf{1}_x, \tag{3b.15}$$

where $\gamma'(x) := \langle x|\gamma|x\rangle$ and $\alpha'(x) := \langle x|\alpha'|x\rangle$. Note that the product of any two operators on $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$ of the form $A(x)\mathbf{1}_x$ and $B(x)\mathbf{1}_x$, where A and B are 2×2 matrices as in (3b.15), is given by the operator $(A(x)B(x))\,\mathbf{1}_x$. According to this rule one easily checks that the trace on $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$ of Γ_x^2 satisfies

$$\begin{aligned} \tfrac12\mathrm{Tr}[\Gamma_x'^{\,2}] &= \gamma'(x)^2+|\alpha'(x)|^2+\tfrac12-\gamma'(x) \\ &= [\gamma'(x)-\tfrac12]^2+|\alpha'(x)|^2+\tfrac14. \end{aligned} \tag{3b.16}$$

By means of (3b.16) we may rewrite the pressure functional (3a.8) as

$$\begin{aligned} -\mathcal{P}_{\beta,\mu}(\Gamma') := -\mathcal{P}_{\beta,\mu}(\Gamma) =& 2\mathrm{Tr}[t\gamma]-\tfrac12\sum_x U_x\left(\mathrm{Tr}[\Gamma_x'^{\,2}]+\tfrac12\right) \\ &-2\mu\mathrm{Tr}[\gamma']+\beta^{-1}\mathrm{Tr}[\Gamma'\ln\Gamma'+(\mathbf{1}-\Gamma')\ln(\mathbf{1}-\Gamma')]. \end{aligned} \tag{3b.17}$$

Finally, we embed the hopping matrix into the 2×2-matrix formalism. We define for any real number λ

$$T_\lambda := \begin{pmatrix} t-\lambda & \\ & -(\overline{t}-\lambda) \end{pmatrix}. \tag{3b.18}$$

With this definition we obtain

$$\tfrac12\mathrm{Tr}[T_\lambda\Gamma'] = \mathrm{Tr}[t\gamma']-\lambda\mathrm{Tr}[\gamma']+\tfrac12\lambda|\Lambda|, \tag{3b.19}$$

and, hence,

$$\begin{aligned} -\mathcal{P}_{\beta,\mu}(\Gamma') =& \mathrm{Tr}[T_\mu\Gamma']-\tfrac12\sum_x U_x\mathrm{Tr}[\Gamma_x'^{\,2}] \\ &+\beta^{-1}\mathrm{Tr}[\Gamma'\ln\Gamma'+(\mathbf{1}-\Gamma')\ln(\mathbf{1}-\Gamma')]+\tfrac14\sum_x U_x-\mu|\Lambda|. \end{aligned} \tag{3b.20}$$

We rewrite Γ'_x as

$$\Gamma_x = (\gamma'(x) - \tfrac{1}{2}) \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \mathbf{1}_x + \begin{pmatrix} & \alpha'(x) \\ \overline{\alpha}'(x) & \end{pmatrix} \mathbf{1}_x + \tfrac{1}{2}\mathbf{1}_x. \tag{3b.21}$$

The cross terms in ${\Gamma'_x}^2$ are traceless, which implies that

$$\begin{aligned} \mathrm{Tr}[{\Gamma'_x}^2] &= \mathrm{Tr}[(\Gamma'_x - \tfrac{1}{2}\mathbf{1}_x)^2] + \tfrac{1}{4}\mathrm{Tr}[\mathbf{1}_x] \\ &= \mathrm{Tr}[(\Gamma'_x - \tfrac{1}{2}\mathbf{1}_x)^2] + \tfrac{1}{2}. \end{aligned} \tag{3b.22}$$

Using (3b.22), (3b.20) becomes

$$\begin{aligned} -\mathcal{P}_{\beta,\mu}(\Gamma') = \mathrm{Tr}[T_\mu \Gamma'] - \tfrac{1}{2} \sum_x U_x \mathrm{Tr}[(\Gamma'_x - \tfrac{1}{2}\mathbf{1}_x)^2] \\ - \mu|\Lambda| + \beta^{-1}\mathrm{Tr}[\Gamma' \ln \Gamma' + (\mathbf{1} - \Gamma')\ln(\mathbf{1} - \Gamma')]. \end{aligned} \tag{3b.23}$$

We associate a multiplication operator $UD := \sum_x U_x D_x \mathbf{1}_x$ with any real function $d(x)$ and complex function $\delta(x)$ by

$$D_x = \begin{pmatrix} d(x) & \delta(x) \\ \overline{\delta(x)} & -d(x) \end{pmatrix}. \tag{3b.24}$$

Notice that D_x has the same form as $\Gamma'_x - \frac{1}{2}\mathbf{1}_x$. The operator UD is really a matrix-valued potential which will enable us to linearize the quadratic trace in (3b.23) by means of the identity

$$\begin{aligned} -\mathrm{Tr}[(\Gamma'_x - \tfrac{1}{2}\mathbf{1}_x)^2] &= \min_{d,\delta} \big\{ -2\mathrm{Tr}[D_x(\Gamma'_x - \tfrac{1}{2}\mathbf{1}_x)] + \mathrm{Tr}[D_x^2] \big\} \\ &= \min_{d,\delta} \big\{ -2\mathrm{Tr}[D_x \Gamma'_x] + \mathrm{Tr}[D_x^2] \big\}. \end{aligned} \tag{3b.25}$$

Indeed it is possible to convert the variation over 1-*pdm*'s in (3a.9) into a variation over all matrix-valued potentials D, which we will show by means of the following lemma.

3.2 LEMMA: *Let D be any matrix-valued potential as in (3b.24), Q be a self-adjoint operator on $\mathcal{H}_\Lambda \oplus \mathcal{H}_\Lambda$ and V the unitary given by*

$$V := \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}. \tag{3b.26}$$

Suppose that F is an odd real-valued function, i.e., $F[x] = -F[-x]$. Then $\widetilde{\Gamma}$ defined by

$$\widetilde{\Gamma} - \tfrac{1}{2} := F\,[T_\mu - UD] + Q - V\overline{Q}V^\dagger, \tag{3b.27}$$

fulfills (3b.13), (3b.14).

Proof: It is easily checked that $VT_\mu V^\dagger = -\overline{T}_\mu$ and $VUDV^\dagger = -\overline{UD}$. Then by the spectral theorem,

$$\begin{aligned} V(\widetilde{\Gamma} - \tfrac{1}{2})V^\dagger &= F\,\big[V(T_\mu - UD)V^\dagger\big] + VQV^\dagger - \overline{Q} \\ &= F\,\big[-(\overline{T_\mu - UD})\big] - (\overline{Q - V\overline{Q}V^\dagger}) \\ &= -\,\overline{\big(F\,[T_\mu - UD] + Q - V\overline{Q}V^\dagger\big)} \\ &= -\,(\overline{\widetilde{\Gamma} - \tfrac{1}{2}}), \end{aligned} \tag{3b.28}$$

which is equivalent to (3b.13) and (3b.14). ■

3.3 THEOREM (Positive temperature pressure): *For all $0 < \beta < \infty$ and all μ we can write the pressure $\mathcal{P}(\beta, \mu)$ as the following variation over the functions d and δ.*

$$-\mathcal{P}(\beta,\mu) = \min_{d,\delta} \mathcal{R}_{\beta,\mu}(d,\delta) - \left(2\beta^{-1}\ln 2 + \mu\right)|\Lambda|, \tag{3b.29}$$

where

$$\mathcal{R}_{\beta,\mu}(d,\delta) := \mathcal{R}_{\beta,\mu}(D) := -\beta^{-1}\mathrm{Tr}[\ln\cosh\tfrac{\beta}{2}(T_\mu - UD)] + \tfrac{1}{2}\sum_x U_x \mathrm{Tr}[D_x^2]. \tag{3b.30}$$

If a potential D minimizes $\mathcal{R}_{\beta,\mu}$ then the operator

$$\Gamma' = \left(\mathbf{1} + \exp\Big[\beta(T_\mu - UD)\Big]\right)^{-1}, \tag{3b.31}$$

is a minimizer for (3b.23), (i.e., defines a HF Gibbs state) and satisfies the consistency equation

$$\Gamma'_x = \left(D_x + \tfrac{1}{2}\right)\mathbf{1}_x. \tag{3b.32}$$

Conversely, if Γ' is a minimizer for (3b.23) then the potential D defined by (3b.32) minimizes $\mathcal{R}_{\beta,\mu}$ and satisfies (3b.31).

Proof: By means of (3b.25) we write

$$\begin{aligned}-\mathcal{P}(\beta,\mu) &= \min_{\Gamma'}\min_{d,\delta}\Bigg\{\mathrm{Tr}[(T_\mu - UD)\Gamma'] + \tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2] \\ &\qquad - \mu|\Lambda| + \beta^{-1}\mathrm{Tr}[\Gamma'\ln\Gamma' + (\mathbf{1}-\Gamma')\ln(\mathbf{1}-\Gamma')]\Bigg\} \\ &= \min_{d,\delta}\Bigg\{\min_{\Gamma'}\Big\{\mathrm{Tr}[(T_\mu - UD)\Gamma'] + \beta^{-1}\mathrm{Tr}[\Gamma'\ln\Gamma' + (\mathbf{1}-\Gamma')\ln(\mathbf{1}-\Gamma')]\Big\} \\ &\qquad + \tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2]\Bigg\} - \mu|\Lambda|. \end{aligned} \tag{3b.33}$$

The minimum is over all $0 \le \Gamma' \le \mathbf{1}$ satisfying (3b.13) and (3b.14). Note that all we did in (3b.33) was to interchange the two minimizations this is of course allowed since we are simply looking for the minimum in the set of all Γ', d and δ.

First relaxing the minimization to be over all $0 \le \Gamma' \le \mathbf{1}$, we can explicitly compute the minimum over Γ' in the second line in (3b.33). We see that the minimum is uniquely achieved for the Γ' defined in (3b.31). We observe, however, that $\Gamma' - \frac{1}{2} = -\frac{1}{2}\tanh\beta(T_\mu - UD)$ is of the form suitable for Lemma 3.2 (choosing $F[x] = -\frac{1}{2}\tanh[\beta x]$ and $Q = 0$). The operator Γ' defined by (3b.31) therefore automatically satisfies (3b.13) and (3b.14) and we have, indeed, found the minimizer in the second line in (3b.33). Moreover, a simple computation then shows that the right side of (3b.33) is identical to the left side of (3b.29).

If D minimizes $\mathcal{R}_{\beta,\mu}$ and we define Γ' by (3b.31) we have from (3b.25) and (3b.29) that

$$\begin{aligned}-\mathcal{P}(\beta,\mu)=\mathcal{R}_{\beta,\mu}(D)-(2\beta^{-1}\ln 2+\mu)|\Lambda| =&\mathrm{Tr}[(T_\mu-UD)\Gamma']+\tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2]\\ &-\mu|\Lambda|+\beta^{-1}\mathrm{Tr}[\Gamma'\ln\Gamma'+(\mathbf{1}-\Gamma')\ln(\mathbf{1}-\Gamma')]\\ \geq&-\mathcal{P}_{\beta,\mu}(\Gamma').\end{aligned} \tag{3b.34}$$

Since $-\mathcal{P}(\beta,\mu)\leq-\mathcal{P}_{\beta,\mu}(\Gamma')$ we must have equality in (3b.34) but it follows from (3b.25) that this can only happen if (3b.32) holds.

Conversely, if Γ' minimizes $-\mathcal{P}_{\beta,\mu}$ and we define D by (3b.32) we see that

$$\begin{aligned}-\mathcal{P}(\beta,\mu)=-\mathcal{P}_{\beta,\mu}(\Gamma') =&\mathrm{Tr}[(T_\mu-UD)\Gamma']+\tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2]\\ &-\mu|\Lambda|+\beta^{-1}\mathrm{Tr}[\Gamma'\ln\Gamma'+(\mathbf{1}-\Gamma')\ln(\mathbf{1}-\Gamma')]\\ \geq&\mathcal{R}_{\beta,\mu}(D)-(2\beta^{-1}\ln 2+\mu)|\Lambda|\end{aligned} \tag{3b.35}$$

and we conclude that D is a minimizer for $\mathcal{R}_{\beta,\mu}$ and that (3b.31) must hold. ■

We remark that the minimum of $\mathcal{R}_{\beta,\mu}(d,\delta)$ will be attained for d and δ satisfying

$$d(x)^2+|\delta(x)|^2\leq\tfrac{1}{4}\quad\text{for all } x\in\Lambda. \tag{3b.36}$$

In fact, since $0\leq\Gamma'\leq\mathbf{1}$ we see from (3b.32) that $D_x^2\leq\frac{1}{4}$ which implies (3b.36).

III.c GAP AND ZERO TEMPERATURE LIMIT

Our discussion will turn in this section to the zero temperature limit $\beta\to\infty$. Recall that the generalized HF energy is given by

$$E^{\mathrm{HF}}(\mu)=\inf\{\mathcal{E}(\Gamma')-\mu N(\Gamma')\ \mid\ \Gamma'\ \text{is a 1-}pdm\}. \tag{3c.1}$$

A minimizing 1-*pdm* Γ'_0, that is one that satisfies, $E^{\mathrm{HF}}(\mu)=\mathcal{E}(\Gamma'_0)-\mu N(\Gamma'_0)$, is called a HF ground state. To make contact with our previous notation let us denote

$$-\mathcal{P}_{\infty,\mu}(\Gamma'):=\mathcal{E}(\Gamma')-\mu N(\Gamma')=\lim_{\beta\to\infty}-\mathcal{P}_{\beta,\mu}(\Gamma'), \tag{3c.2}$$

and $-\mathcal{P}(\infty,\mu):=E^{\mathrm{HF}}(\mu)=\lim_{\beta\to\infty}-\mathcal{P}(\beta,\mu)$.

We can derive an analog of Theorem 3.3 for the zero temperature pressure by simply dropping the term $-\beta^{-1}S(\Gamma)$, and essentially repeating the whole positive temperature discussion. There is, however, one subtle difference. Given the potential D, the minimizing Γ' in (3b.33) was uniquely defined by (3b.31). In the zero temperature case the Γ' we are looking for is simply the minimizer of $\mathrm{Tr}[(T_\mu-UD)\Gamma']$. If the operator $(T_\mu-UD)$ has zero eigenvalues this minimizer would not be uniquely defined. In our case, however, we prove in Lemma 3.5 below that $(T_\mu-UD)$ has no zero eigenvalues. In fact,

$$|e_j|\geq\tfrac{1}{4}\min_x\{U_x\}|\Lambda|^{-1}>0$$

for any eigenvalue e_j of $T_\mu-UD$. We can therefore write that the minimizer of $\mathrm{Tr}[(T_\mu-UD)\Gamma']$ is $\Gamma'=\chi(T_\mu-UD)=\lim_{\beta\to\infty}(\mathbf{1}+\exp[\beta(T_\mu-UD)])^{-1}$, where $\chi(a):=1$ if $a<0$ and zero otherwise. The point is that the value $\chi(0)$ is unimportant. Let us note that there is another way of characterizing the zero temperature states, thereby avoiding the repetition of the whole positive temperature discussion. Namely, the main theorem 3.12 of this chapter allows us to obtain all zero temperature states as limits of positive temperature states.

3.4 THEOREM (Ground state pressure): *We have*

$$-\mathcal{P}(\infty,\mu) = E^{\mathrm{HF}}(\mu) = \min_{d,\delta} \mathcal{R}_{\infty,\mu}(d,\delta) - \mu|\Lambda|,$$

where

$$\mathcal{R}_{\infty,\mu}(d,\delta) := \mathcal{R}_{\infty,\mu}(D) := -\tfrac{1}{2}\mathrm{Tr}|T_\mu - UD| + \tfrac{1}{2}\sum_x U_x \mathrm{Tr}[D_x^2]. \tag{3c.3}$$

If a potential D minimizes $\mathcal{R}_{\infty,\mu}$ then the operator (with χ defined as above)

$$\Gamma' = \chi(T_\mu - UD), \tag{3c.4}$$

minimizes (3c.2), (i.e., defines a HF ground state) and satisfies the consistency equation

$$\Gamma'_x = (D_x + \tfrac{1}{2})\mathbf{1}_x. \tag{3c.5}$$

Conversely, if Γ' minimizes (3c.2) then the potential D defined by (3c.5) minimizes $\mathcal{R}_{\infty,\mu}$ and satisfies (3c.4).

The reader may wonder why the pressure depends on the absolute value of $T_\mu - UD$ and not only on the negative eigenvalues. In this context it should be kept in mind that because of the special form of the operator $T_\mu - UD$ the trace $-\frac{1}{2}\mathrm{Tr}|T_\mu - UD|$ is, in fact, equal to the sum of the negative eigenvalues. In comparing (3c.3) to (3b.30) we notice that $\lim_{\beta\to\infty}\beta^{-1}\ln\cosh(\beta x/2) = \frac{1}{2}|x|$ it is therefore natural to write the absolute value in (3c.3). It remains to prove the absence of zero eigenvalues.

3.5 LEMMA (Gap estimate): *Let D be a minimizing matrix-valued potential for $\mathcal{R}_{\beta,\mu}$ with $0 < \beta \le \infty$ and denote the eigenvalues of $T_\mu - UD$ by $e_1, e_2, \ldots, e_{2|\Lambda|}$. Then, for any $j = 1, 2, \ldots, 2|\Lambda|$, we have*

$$|e_j| \ge \tfrac{1}{4}U_{\min}|\Lambda|^{-1} - \beta^{-1}2\ln 2, \tag{3c.6}$$

where $U_{\min} := \min_{x\in\Lambda}\{U_x\}$.

Proof: If D minimizes $\mathcal{R}_{\beta,\mu}$ for finite β we know that the operator Γ' defined in (3b.31) minimizes the functional $-\mathcal{P}_{\beta,\mu}$ in (3b.23). Likewise, if D minimizes $\mathcal{R}_{\infty,\mu}$ we know that the operator $\Gamma' = \lim_{\beta\to\infty}(\mathbf{1} + \exp[\beta(T_\mu - UD)])^{-1}$ minimizes the energy functional (3c.2). Notice that these definitions of Γ' imply (3b.13) and (3b.14). What we do not know a-priori is that if $\beta = \infty$ (i.e., zero temperature), then Γ' agrees with $\chi(T_\mu - UD)$.

Let $Q := |\varphi\rangle\langle\varphi|$ denote the projection onto some eigenvector φ of $T_\mu - UD$ with corresponding eigenvalue e. Note that $V\overline{Q}V^\dagger$ is the projection onto the eigenvector $V\overline{\varphi}$ of $T_\mu - UD$ with eigenvalue $-e$, provided V is the unitary given by (3b.26).

In terms of the operators Γ' discussed above we define

$$\widetilde{\Gamma}' := \Gamma' + \delta Q - \delta V\overline{Q}V^\dagger. \tag{3c.7}$$

We choose $-1/2 \le \delta \le 1/2$ such that $e\delta \ge 0$. With this choice $0 \le \widetilde{\Gamma}' \le \mathbf{1}$. Note that φ is an eigenvector of Γ'. We denote its eigenvalue by λ. Then φ is also an eigenvector of $\widetilde{\Gamma}'$ with eigenvalue $\lambda + \delta$. With our choice of δ we have $0 \le \lambda, \lambda+\delta \le 1$.

Lemma 3.2 now implies that $\widetilde{\Gamma}'$ is admissible on $\mathcal{H}_\Lambda \oplus \mathcal{H}_\Lambda$, as it corresponds to the 1-*pdm*

$$Y^\dagger \begin{pmatrix} \widetilde{\Gamma}' & \\ & \widetilde{\Gamma}' \end{pmatrix} Y. \tag{3c.8}$$

Since Γ' minimizes $-\mathcal{P}_{\beta,\mu}$ it follows that

$$\begin{aligned} 0 \ge & \mathcal{P}_{\beta,\mu}(\widetilde{\Gamma}') - \mathcal{P}_{\beta,\mu}(\Gamma') \\ = & -\delta \mathrm{Tr}[T_\mu(Q - V\overline{Q}V^\dagger)] - \tfrac{1}{2}\sum_x U_x \mathrm{Tr}[(\Gamma'_x - \tfrac{1}{2}\mathbf{1}_x)^2 - (\Gamma'_x - \tfrac{1}{2}\mathbf{1}_x + \delta Q_x - \delta V \overline{Q}_x V^\dagger)^2] \\ & + 2\beta^{-1}[\lambda \ln \lambda + (1-\lambda)\ln(1-\lambda) - (\lambda+\delta)\ln(\lambda+\delta) - (1-\lambda-\delta)\ln(1-\lambda-\delta)] \\ = & -2\delta e + \tfrac{1}{2}\delta^2 \sum_x U_x \mathrm{Tr}[(Q_x - V\overline{Q}_x V^\dagger)^2] + 2\beta^{-1}[f(\lambda) - f(\lambda+\delta)], \end{aligned} \tag{3c.9}$$

where $f(\lambda) := \lambda \ln \lambda + (1-\lambda)\ln(1-\lambda)$. Clearly, $-\ln 2 \le f(\lambda) \le 0$ for $0 \le \lambda \le 1$. Hence $|f(\lambda) - f(\lambda+\delta)| \le \ln 2$. We insert this estimate into (3c.9) and obtain, using $\delta e = |\delta||e|$

$$2|e| \ge \tfrac{1}{2}|\delta| \sum_x U_x \mathrm{Tr}[(Q_x - V\overline{Q}_x V^\dagger)^2] - 2|\delta|^{-1}\beta^{-1}\ln 2. \tag{3c.10}$$

Furthermore,

$$\mathrm{Tr}[(Q_x - V\overline{Q}_x V^\dagger)^2] = 2\left(|\varphi(x,\uparrow)|^2 + |\varphi(x,\downarrow)|^2\right)^2, \tag{3c.11}$$

leads us by the Schwarz inequality to

$$\begin{aligned} \sum_x U_x \mathrm{Tr}[(Q_x - V\overline{Q}_x V^\dagger)^2] \ge & 2U_{\min} \sum_x \left(|\varphi(x,\uparrow)|^2 + |\varphi(x,\downarrow)|^2\right)^2 \\ \ge & 2U_{\min}|\Lambda|^{-1} \left(\sum_x |\varphi(x,\uparrow)|^2 + |\varphi(x,\downarrow)|^2\right)^2 \\ = & 2U_{\min}|\Lambda|^{-1}. \end{aligned} \tag{3c.12}$$

Inserting (3c.12) into (3c.10) and choosing $|\delta| = \frac{1}{2}$ concludes the proof. ∎

We interpret any minimizing Γ in Theorems 3.3 and 3.4 as the physical state of the system at β, μ. Since Γ, subject to (3b.31), is the Fermi distribution of the corresponding operator $T_\mu - UD$, we might as well interpret its eigenstates as the only orbitals the electrons can possibly occupy. This is nothing but viewing $T_\mu - UD$ as the relevant quasiparticle Hamiltonian for the considered system. From the BCS theory of superconductivity the question arises whether or not the quasiparticle spectrum, i. e., the spectrum of $T_\mu - UD$ has a gap around 0 for low enough temperatures. The answer to this question is always positive as we have just pointed out in Lemma 3.5. We remark, however, that our estimate for the size of the gap becomes trivial in the thermodynamic limit. In Theorem 3.15 below we give a formula for the gap in the translation invariant case.

III.d BROKEN GAUGE SYMMETRIES

We pause to remark that so far no assumption was made about the hopping matrix t, except that it be self-adjoint, connected and traceless. In Theorems 3.3 and 3.4 in the previous section we established a unique correspondence between the HF ground and Gibbs states (described by Γ') and the potentials D that minmize $\mathcal{R}_{\beta,\mu}$. We can therefore now entirely concentrate on the determination of the functions d and δ that yield a minimizer D for $\mathcal{R}_{\beta,\mu}$, where $0<\beta\leq\infty$.

A key ingredient in the following analysis are the representations

$$\begin{aligned}\ln\cosh x =& \sum_{k=0}^{\infty}\ln\left[1+\left(\frac{x}{\pi(k+1/2)}\right)^2\right],\\ |x| =& \frac{1}{\pi}\int_0^{\infty}\ln\left(1+\frac{x^2}{c^2}\right)dc.\end{aligned} \tag{3d.1}$$

The significance of (3d.1), as examples of *integrated Pick functions*, was emphasized in Lieb and Loss [LL] and Kennedy and Lieb [KL]. The virtue of (3d.1) is, roughly speaking, that it allows us to convert traces into determinants. In fact, using these representations we may write

$$\begin{aligned}\mathcal{R}_{\beta,\mu}(D) =& -\beta^{-1}\sum_{k=0}^{\infty}\Big[\ln\mathrm{Det}\{4\pi^2(k+1/2)^2\beta^{-2}+(T_\mu-UD)^2\}\\ &\qquad -2|\Lambda|\ln\{4\pi^2(k+1/2)^2\beta^{-2}\}\Big]+\tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2],\end{aligned} \tag{3d.2}$$

$$\begin{aligned}\mathcal{R}_{\infty,\mu}(D) =& -\frac{1}{\pi}\int_0^{\infty}\Big[\tfrac{1}{2}\ln\mathrm{Det}\{c^2+(T_\mu-UD)^2\}-2|\Lambda|\ln c\Big]dc\\ &+\tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2].\end{aligned} \tag{3d.3}$$

Since we are dealing with finite dimensional matrices, convergence of the above expressions are evident for any choice of D.

3.6 LEMMA (Phase alignment): *Let t be real. Then,*

$$\mathcal{R}_{\beta,\mu}(d,\delta)\geq\mathcal{R}_{\beta,\mu}(d,e^{i\theta}|\delta|). \tag{3d.4}$$

If $\delta(x)\neq0$ for all $x\in\Lambda$, equality holds in (3d.4) only if $\delta(x)=|\delta(x)|e^{i\theta}$ for all points $x\in\Lambda$ and for some fixed $0\leq\theta<2\pi$.

Remark: Lemma 3.8 below will show that, for the ground state, either $\delta(x)\neq0$ for all x or else $\delta(x)=0$ for all x.

Proof: In order to prove (3d.4) we may assume that $\delta(x)\neq0$ for all $x\in\Lambda$. In fact, if we have proved (3d.4) for non-vanishing δ we conclude for general δ by the continuity of $\mathcal{R}_{\beta,\mu}$ that

$$\mathcal{R}_{\beta,\mu}(d,\delta)=\lim_{\varepsilon\to0}\mathcal{R}_{\beta,\mu}(d,\delta+\varepsilon)\geq\lim_{\varepsilon\to0}\mathcal{R}_{\beta,\mu}(d,|\delta+\varepsilon|)=\mathcal{R}_{\beta,\mu}(d,|\delta|). \tag{3d.5}$$

For the cases of equality, however, we have to assume δ non-vanishing.

Just as D corresponds to d and δ via (3b.24), we denote the operator corresponding to $\widetilde{d}=d$ and $\widetilde{\delta}:=e^{i\theta}|\delta|$ by $\widetilde{D}$. In view of (3d.2–3), it suffices to prove, for every real c, that

$$\ln\mathrm{Det}[c^2+(T_\mu-UD)^2]\leq\ln\mathrm{Det}[c^2+(T_\mu-U\widetilde{D})^2] \tag{3d.6}$$

and to show that equality in (3d.6) implies $\delta(x) = e^{i\theta}|\delta(x)|$ for some $0 \le \theta < 2\pi$.

To this end, we define an operator

$$B := \sum_x B_x, \tag{3d.7}$$

with $B_x > 0$ (to be chosen below). Furthermore, we rewrite UD in the following way. Let $F := \sum_x F_x \mathbf{1}_x$ and $G := \sum_x G_x \mathbf{1}_x$, where

$$\begin{aligned} F_x &:= U_x \; d(x) \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}, \\ G_x &:= U_x \begin{pmatrix} & \delta(x) \\ \overline{\delta(x)} & \end{pmatrix}. \end{aligned} \tag{3d.8}$$

Hence,

$$T_\mu - UD = T_\mu - F - G. \tag{3d.9}$$

Notice that both F and G commute with B, and that F and G anticommute. Thus, abbreviating $B^{1/2} Q B^{1/2} =: \widehat{Q}$ for any operator Q we have the following identity.

$$\begin{aligned} &\ln \operatorname{Det}[c^2 + (T_\mu - UD)^2] + 2 \ln \operatorname{Det}[B] \\ &\quad = \ln \operatorname{Det}[B^{1/2}(ic + T_\mu - F - G) B (-ic + T_\mu - F - G) B^{1/2}] \\ &\quad = \ln \operatorname{Det}[A(c, D) - \{\widehat{T}_\mu, \widehat{G}\}], \end{aligned} \tag{3d.10}$$

where $\{A, B\} := AB + BA$ is the anticommutator and where

$$A(c, D) := c^2 B^2 + (\widehat{T}_\mu - \widehat{F})^2 + \widehat{G}^2 + ic[B, \widehat{T}_\mu]. \tag{3d.11}$$

We shall now prove that

$$\ln \operatorname{Det}[c^2 + (T_\mu - UD)^2] \le \ln \operatorname{Det}[A(c, D)] - 2 \ln \operatorname{Det}[B], \tag{3d.12}$$

and that equality holds in (3d.12) if and only if $\{\widehat{T}_\mu, \widehat{G}\}$ vanishes.

We will prove this claim by using a concavity argument. Introducing a unitary

$$V := \begin{pmatrix} 0 & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}, \tag{3d.13}$$

one easily checks that $VBV^\dagger = B$, $V\widehat{T}_\mu V^\dagger = -\widehat{T}_\mu = -\overline{\widehat{T}_\mu}$, using the reality of t, and $VFV^\dagger = -F$, $VGV^\dagger = \overline{G}$. Hence, we obtain

$$VA(c, D)V^\dagger = A(-c, D) = \overline{A(-c, D)}, \qquad V\{\widehat{T}_\mu, \widehat{G}\}V^\dagger = -\overline{\{\widehat{T}_\mu, \widehat{G}\}} \tag{3d.14}$$

Now, from (3d.10) we see that the determinant in question is real and depends only on c^2. Therefore,

$$\begin{aligned} &\ln \operatorname{Det}[A(c, D) - \{\widehat{T}_\mu, \widehat{G}\}] = \ln \operatorname{Det}[A(-c, D) - \{\widehat{T}_\mu, \widehat{G}\}] \\ &\quad = \ln \operatorname{Det}[\overline{A(-c, D)} - \overline{\{\widehat{T}_\mu, \widehat{G}\}}] = \ln \operatorname{Det}[V(A(c, D) + \{\widehat{T}_\mu, \widehat{G}\})V^\dagger] \\ &\quad = \ln \operatorname{Det}[A(c, D) + \{\widehat{T}_\mu, \widehat{G}\}]. \end{aligned} \tag{3d.15}$$

By the strict concavity of $\ln\mathrm{Det}[\cdot]$, i.e., $\frac{1}{2}\ln\mathrm{Det}[a]+\frac{1}{2}\ln\mathrm{Det}[b]\leq\ln\mathrm{Det}[\frac{1}{2}(a+b)]$, with strict inequality unless $a=b$, we arrive at the assertion in (3d.12).

We now choose $B_x=U_x^{-1}|\delta(x)|^{-1}$, keeping in mind our assumptions that $\delta(x)\neq 0$ and $U_x>0$. The key observation is that

$$\widehat{G}_x=(BG)_x=\frac{1}{|\delta(x)|}\begin{pmatrix} & \delta(x)\\ \overline{\delta(x)} & \end{pmatrix} \tag{3d.16}$$

is unitary for all $x\in\Lambda$, i.e., $B^2G^2=\mathbf{1}$. Thus, for any two points $x,y\in\Lambda$ the 2×2 matrices belonging to $(\widehat{G})_x$ and $(\widehat{G})_y$ are identical modulo a phase factor $\delta(x)\overline{\delta(y)}|\delta(x)\delta(y)|^{-1}$. The last term $\{\widehat{T}_\mu,\widehat{G}\}$ vanishes if and only if

$$t_{xy}\delta(x)|\delta(x)|^{-1}=t_{xy}\delta(y)|\delta(y)|^{-1} \tag{3d.17}$$

for all $x,y\in\Lambda$. It is essential for (3d.17) that t be real. From (3d.17) we learn by the connectedness of t that $\widehat{T}_\mu\widehat{G}+\widehat{G}\widehat{T}_\mu$ vanishes if and only if δ is of the desired form, $\delta(x)=e^{i\theta}|\delta(x)|$.

Notice now that $A(c,D)=A(c,\tilde{D})$ and that for $\tilde{D}$ we have equality in (3d.12). Inequality (3d.6) is therefore a consequence of (3d.12). ■

We remark that by (3d.12) we also get a lower bound on $\mathcal{R}_{\beta,\mu}(D)$ that depends only on d and $|\delta|$, even in cases in which t is not real. However, this lower bound cannot then be expressed as $\mathcal{R}_{\beta,\mu}(D')$ for some matrix-valued potential D'. The reason is that (3d.17) now reads $t_{xy}\delta(x)|\delta(x)|^{-1}=\overline{t_{xy}}\delta(y)|\delta(y)|^{-1}$. This equation cannot be satisfied unless $\delta\equiv 0$ as shown in (3d.26) below.

The strategy for proving Lemma 3.6 can actually be applied to other types of hopping matrices, as the following lemma shows. Using the notion of pseudo-spin discussed below (in (3d.50–53)) the conclusion of the next lemma is that minimizers will have aligned pseudo-spin.

3.7 LEMMA (Pseudo-spin alignment): *Let t be bipartite (but not necessarily real) and $\mu=0$. Then*

$$\mathcal{R}_{\beta,0}(d,\delta)\geq\mathcal{R}_{\beta,0}\left((-1)^x\sqrt{d^2+|\delta|^2},0\right). \tag{3d.18}$$

In case t is not real and $n(x):=\sqrt{d^2(x)+|\delta(x)|^2}\neq 0$ for all $x\in\Lambda$ equality holds in (3d.18) if and only if $\delta(x)=0$ and $d(x)=(-1)^x n(x)$ or $d(x)=(-1)^x n(x)$ for all $x\in\Lambda$. In case t is real and $n(x)\neq 0$ for all $x\in\Lambda$ equality holds in (3d.18) if and only if for all $x\in\lambda$

$$\begin{pmatrix} d(x) & \delta(x)\\ \overline{\delta}(x) & -d(x)\end{pmatrix}=w_x\begin{pmatrix}(-1)^x n(x) & \\ & -(-1)^x n(x)\end{pmatrix}w_x^\dagger, \tag{3d.19}$$

where

$$w_x=\begin{pmatrix}(-1)^x & \\ & 1\end{pmatrix}w\begin{pmatrix}(-1)^x & \\ & 1\end{pmatrix}$$

for some unitary 2×2-matrix w independent of $x\in\Lambda$.

Proof: Since the main idea of the proof is the same as that in Lemma 3.6, we shall use the notation therein. In proving (3d.18) we can assume $n(x)$ non-vanishing for all x, otherwise we use a continuity argument as in Lemma 3.6. For simplicity we write $T_{\mu=0}=T$. Again, our assertion follows by showing that for all real numbers c the inequality

$$\ln\mathrm{Det}[c^2+(T-UD)^2]\geq\ln\mathrm{Det}[c^2+(T-U\widetilde{D})^2] \tag{3d.20}$$

holds, and there is equality if and only if d and δ fulfill (3d.19) and $\widetilde{D}$ is assumed to be some matrix-valued potential for which the corresponding functions $\widetilde{d}$ and $\widetilde{\delta}$ do obey (3d.19).

Again, we define $\widehat{Q} := B^{1/2}QB^{1/2}$. In analogy with (3d.10) we obtain

$$\begin{aligned}&\ln \mathrm{Det}[c^2 + (T-UD)^2] + 2\ln \mathrm{Det}[B]\\ &\quad= \ln \mathrm{Det}[B^{1/2}(ic+T-UD)B(-ic+T-UD)B^{1/2}]\\ &\quad= \ln \mathrm{Det}[A_*(c,D) - \{\widehat{T}, U\widehat{D}\}],\end{aligned} \tag{3d.21}$$

where now

$$A_*(c,D) := (U\widehat{D})^2 + c^2B^2 + \widehat{T}^2 + ic[B,\widehat{T}]. \tag{3d.22}$$

Thanks to our assumption of bipartiteness of t and the special choice of $\mu = 0$ for all $x \in \Lambda$, we can now repeat the concavity argument above, using the unitary $(-1)^x$. Indeed, $(-1)^x\widehat{T}(-1)^x = -\widehat{T}$, $(-1)^xB(-1)^x = B$, $(-1)^xUD(-1)^x = UD$, $(-1)^xA_*(-c,D)(-1)^x = A_*(c,D)$, and thus

$$\ln \mathrm{Det}[A_*(c,D) - \{\widehat{T}, U\widehat{D}\}] = \ln \mathrm{Det}[A_*(-c,D) - \{\widehat{T}, U\widehat{D}\}] = \ln \mathrm{Det}[A_*(c,D) + \{\widehat{T}, U\widehat{D}\}], \tag{3d.23}$$

Hence, concavity of $\ln \mathrm{Det}[\cdot]$ again implies that

$$\ln \mathrm{Det}[c^2 + (T-UD)^2] \le \ln \mathrm{Det}[A_*(c,D)] - 2\ln \mathrm{Det}[B] \tag{3d.24}$$

with equality if and only if $\{\widehat{T}, U\widehat{D}\} = 0$. We now make the choice $B_x = {U_x}^{-1}n(x)^{-1}$. The condition $\{\widehat{T}, U\widehat{D}\} = 0$ becomes

$$d(x)/n(x) = -d(y)/n(y) \qquad \text{for } x \in A, y \in B, \tag{3d.25a}$$

$$t_{xy}\delta(x)/n(x) = \overline{t_{xy}}\delta(y)/n(y) \qquad \text{for } x \in A, y \in B. \tag{3d.25b}$$

But (3d.25) is equivalent to (3d.19) provided t is real. Conversely, in case t is not real, as we pointed out in the definition of the hopping matrix, there exists at least one closed path $\{x, x_1, \ldots x_n, x\}$ such that $t_{xx_1}\ldots t_{x_nx}$ is not real. Thus, iterating (3d.25b) along this closed path we obtain

$$\frac{t_{xx_1}\ldots t_{x_nx_1}}{\overline{t}_{xx_1}\ldots \overline{t}_{x_nx_1}}\frac{\delta(x)}{n(x)} = \frac{\delta(x)}{n(x)}, \tag{3d.26}$$

whose only solution is $\delta(x) = 0$, implying $\delta \equiv 0$ on the entire lattice Λ because t is connected. Finally, we remark that we may achieve the bound in (3d.20) by choosing $\widetilde{d}(x) = (-1)^x n(x)$ and $\widetilde{\delta}(x) = 0$. ■

In order to use Lemma 3.6 to conclude that a potential D minimizing $\mathcal{R}_{\beta,\mu}$ is phase aligned we must show that for such a potential $\delta(x) \neq 0$ for all x (or otherwise vanishes everywhere). Likewise, in order to use Lemma 3.7 we must show that a minimizing potential has $n(x) \neq 0$ for all x. We prove these two results in parts (a) and (b) of the next lemma, again using the method of choosing an appropriate normalizer, B.

3.8 LEMMA (Nonvanishing of minimizers): *(a) If t is real and if $D = (d,\delta)$ minimizes $\mathcal{R}_{\beta,\mu}$ then either $\delta(x) \neq 0$ for all x or $\delta(x) = 0$ for all x.*

(b) If $t - \mu$ is bipartite (but not necessarily real) and if $D = (d,\delta)$ minimizes $\mathcal{R}_{\beta,\mu}$ then either $n(x) \neq 0$ for all x or $n(x) = 0$ for all x.

Proof: (a) Let $D=(d,\delta)$ be a potential such that both sets

$$\Lambda_0=\{x\in\Lambda \mid \delta(x)=0\} \quad \text{and} \quad \Lambda\setminus\Lambda_0=\{x\in\Lambda \mid \delta(x)\neq 0\}$$

are non-empty. We shall prove that D cannot be minimizing for $\mathcal{R}_{\beta,\mu}$. For $0<\tau\le 1$ we define a new potential D_τ by

$$d_\tau(x)=d(x) \quad \text{and} \quad \delta_\tau(x)=\begin{cases}\sqrt{1-\tau^2}|\delta(x)|, & x\notin\Lambda_0\\ \tau\delta_{\text{av}}, & x\in\Lambda_0\end{cases}, \tag{3d.27}$$

where $\delta_{\text{av}}^2=\left(\sum_{x\in\Lambda_0}U_x\right)^{-1}\sum\limits_{x\notin\Lambda_0}U_x|\delta(x)|^2>0$. We shall show that for τ small enough $\mathcal{R}_{\beta,\mu}(D)>\mathcal{R}_{\beta,\mu}(D_\tau)$.

According to (3d.2–3) we can write

$$\mathcal{R}_{\beta,\mu}(D)=-\int_0^\infty\Big[\ln\mathrm{Det}[c^2+(T_\mu-UD)^2]-4|\Lambda|\ln c\Big]d\mu_\beta(c)+\sum\nolimits_x U_x\mathrm{Tr}[D_x^2], \tag{3d.28}$$

where the measure $d\mu_\beta$ for $\beta<\infty$ is a sum of Dirac delta functions $d\mu_\beta(c)=\sum\limits_{k=0}^{\infty}\beta^{-1}\delta[(2k+1)\pi\beta^{-1}-c]dc$, while for $\beta=\infty$ it is $d\mu_\infty=(2\pi)^{-1}dc$.

We chose δ_{av} to make the last term in $\mathcal{R}_{\beta,\mu}$ independent of τ, i.e., $\sum_x U_x\mathrm{Tr}[D_x^2]=\sum_x U_x\mathrm{Tr}[D_{\tau,x}^2]$. To conclude that $\mathcal{R}_{\beta,\mu}(D)>\mathcal{R}_{\beta,\mu}(D_\tau)$ we must therefore show that for τ small enough

$$\int\limits_0^\infty\Big\{\ln\mathrm{Det}[c^2+(T_\mu-UD)^2]-\ln\mathrm{Det}[c^2+(T_\mu-UD_\tau)^2]\Big\}d\mu_\beta(c)<0 \tag{3d.29}$$

To prove (3d.29) we again appeal to (3d.12). We choose $B_x=U_x^{-1}[\delta_\tau(x)|^{-1}$ and obtain that

$$\ln\mathrm{Det}[c^2+(T_\mu-UD)^2]\le\ln\mathrm{Det}[A(c,D)]-2\ln\mathrm{Det}[B] \tag{3d.30}$$

and

$$\ln\mathrm{Det}[c^2+(T_\mu-UD_\tau)^2]=\ln\mathrm{Det}[A(c,D_\tau)]-2\ln\mathrm{Det}[B]. \tag{3d.31}$$

Since $\{\widehat{T}_\mu,\widehat{G}_\tau\}=0$ (here G_τ is defined as in (3d.8) but with δ replaced by δ_τ) we see from (3d.10) that

$$A(c,D_\tau)=(icB+\widehat{T}_\mu-U\widehat{D}_\tau)(-ic+\widehat{T}_\mu-U\widehat{D}_\tau)$$

and $A(c,D)=A(c,D_\tau)-\mathbf{1}+\widehat{G}^2$. Therefore (3d.30) and (3d.31) imply

$$\begin{aligned}&\ln\mathrm{Det}[c^2+(T_\mu-UD)^2]-\ln\mathrm{Det}[c^2+(T_\mu-UD_\tau)^2]\\ &\quad\le\ln\mathrm{Det}[\mathbf{1}-(icB+\widehat{T}_\mu-U\widehat{D}_\tau)^{-1}(\mathbf{1}-\widehat{G}^2)(-icB+\widehat{T}_\mu-U\widehat{D}_\tau)^{-1}]\\ &\quad=\mathrm{Tr}\ln[\mathbf{1}-(icB+\widehat{T}_\mu-U\widehat{D}_\tau)^{-1}(\mathbf{1}-\widehat{G}^2)(-icB+\widehat{T}_\mu-U\widehat{D}_\tau)^{-1}].\end{aligned} \tag{3d.32}$$

Using the inequality $\ln(\mathbf{1}-A)\le -A$ we obtain

$$\begin{aligned}&\ln\det[c^2+(T_\mu-UD)^2]-\ln\mathrm{Det}[c^2+(T_\mu-UD_\tau)^2]\\ &\le-\mathrm{Tr}[(icB+\widehat{T}_\mu-U\widehat{D}_\tau)^{-1}(\mathbf{1}-\widehat{G}^2)(-icB+\widehat{T}_\mu-U\widehat{D}_\tau)^{-1}]\\ &\le-\mathrm{Tr}[K_\tau(c)],\end{aligned} \tag{3d.33}$$

where we have denoted

$$
\begin{aligned}
K_\tau(c) :=& (icB+\widehat{T}_\mu - U\widehat{D}_\tau)^{-1}(\mathbf{1}-\widehat{G}^2)(-icB+\widehat{T}_\mu - U\widehat{D}_\tau)^{-1} \\
=& B^{-1/2}(ic+T_\mu - UD_\tau)^{-1}(B^{-1}-BG^2)(-ic+T_\mu-UD_\tau)^{-1}B^{-1/2}.
\end{aligned}
\tag{3d.34}
$$

The estimate (3d.29) follows if we show that for τ small enough

$$
\int \mathrm{Tr}[K_\tau(c)]d\mu_\beta(c) > 0. \tag{3d.35}
$$

We denote by P_0 the projection onto the sites in Λ_0, i.e., $P_0 = \sum_{x\in\Lambda_0} \mathbf{1}_x$ and $\widetilde{P}_0 = \mathbf{1} - P_0 = \sum_{x\notin\Lambda_0} \mathbf{1}_x$. If we assume $\tau \leq \frac{1}{2}$ we then have

$$
B^{-1} - BG^2 = \sum_{x\in\Lambda_0} \tau U_x \delta_{\mathrm{av}} \mathbf{1}_x - \sum_{x\notin\Lambda_0} \frac{\tau^2}{\sqrt{1-\tau^2}} U_x|\delta(x)|\mathbf{1}_x \geq a\tau P_0 - b\tau^2\widetilde{P}_0, \tag{3d.36}
$$

where a and b are strictly positive constants depending on the values of $|\delta(x)|$ and U_x for all x.

We therefore find

$$
\begin{aligned}
\mathrm{Tr}[K_\tau^{(c)}] \geq& \tau a \mathrm{Tr}[B^{-1/2}(ic+T_\mu-UD_\tau)^{-1}P_0(-ic+T_\mu-UD_\tau)^{-1}B^{-1/2}] \\
&- \tau^2 b \mathrm{Tr}[B^{-1/2}(ic+T_\mu-UD_\tau)^{-1}\widetilde{P}_0(-ic+T_\mu-UD_\tau)^{-1}B^{-1/2}].
\end{aligned}
$$

Since $a'\widetilde{P}_0 \leq B^{-1} \leq b'\mathbf{1}$ for constants a' and b' (again depending only on $|\delta(x)|$ and U_x for all x) we have the estimate, with $|A|^2 = AA^\dagger$,

$$
\mathrm{Tr}[K_\tau^{(c)}] \geq \tau a a' \mathrm{Tr}[|\widetilde{P}_0(ic+T_\mu-UD_\tau)^{-1}P_0|^2] - \tau^2 b b' \mathrm{Tr}[(c^2+(T_\mu-UD_\tau)^2)^{-1}]. \tag{3d.37}
$$

Since the problem is finite dimensional it is clear that the eigenvalues of $T_\mu - UD_\tau$ converge to the eigenvalues of $T_\mu - UD$. Hence, the gap estimate (3c.6) implies that for τ small (depending on U_x, D_x and t_{xy}) there is a constant g_β, satisfying $g_\beta > 0$ for β large enough (in particular for $\beta = \infty$) such that $(T_\mu - UD_\tau)^2 \geq g_\beta^2$. Therefore

$$
[c^2 + (T_\mu - UD_\tau)^2]^{-1} \leq (c^2+g_\beta^2)^{-1}\mathbf{1}. \tag{3d.38}
$$

Recall now that the measure $d\mu_\beta$ appearing in the Pick representation (11.2) is supported away from zero when $\beta < \infty$. It therefore follows from (3d.38) that for small enough τ

$$
\int \mathrm{Tr}\Big[\big(c^2+(T_\mu+UD_\tau)^2\big)^{-1}\Big]d\mu_\beta(c)
$$

is bounded independently of τ for all β.

In order to conclude (3d.35) (and hence the lemma) from (3d.37) it only remains to prove that

$$
\liminf_{\tau\to 0} \int \mathrm{Tr}[|\widetilde{P}_0(ic+T_\mu-UD_\tau)^{-1}P_0|^2]d\mu_\beta(c) \neq 0. \tag{3d.39}
$$

Since t is connected we know that

$$\widetilde{P}_0(ic+T_\mu-UD)P_0=\widetilde{P}_0T_0P_0\neq 0 \quad \text{and} \quad P_0(ic+T_\mu-UD)\widetilde{P}_0=P_0T_0\widetilde{P}_0\neq 0.$$

Therefore we must have $\widetilde{P}_0(ic+T_\mu-UD)^{-1}P_0\neq 0$ (because if we have a matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ with operator valued entries and $c\neq 0$ and $b\neq 0$ then its inverse $\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ must have $\beta\neq 0$ and $\gamma\neq 0$). Since $\lim_{\tau\to 0}\mathrm{Tr}[|\widetilde{P}_0(ic+T_\mu-UD_\tau)^{-1}P_0|^2]=\mathrm{Tr}[|\widetilde{P}_0(ic+T_\mu-UD)^{-1}P_0|^2]$ we obtain by Fatou's Lemma that

$$\liminf_{\tau\to 0}\int \mathrm{Tr}[|\widetilde{P}_0(ic+T_\mu-UD_\tau)^{-1}P_0|^2]d\mu_\beta(c)\geq \int \mathrm{Tr}[|\widetilde{P}_0(ic+T_\mu-UD)^{-1}P_0|^2]d\mu_\beta(c)>0$$

and part (a) follows.

(b) Part (b) is proved in the same way as part (a). We this time choose D_τ with $\delta_\tau(x)=0$ and $d_\tau(x)=(-1)^x n_\tau(x)$, where

$$n_\tau(x)=\begin{cases} \sqrt{1-\tau^2}n(x), & x\notin\Lambda_0 \\ \tau n_{\mathrm{av}}, & x\in\Lambda_0 \end{cases}.$$

Here n_{av} is again defined such that $\sum_x U_x n(x)^2=\sum_x U_x n_\tau(x)^2$. The rest of the proof is identical to the proof of part (a) except that we use (3d.24) instead of (3d.12) and we choose $B_x=U_x n_\tau(x)^{-1}$.■

We pause to discuss the symmetry aspects of the Hubbard model and how they are reflected by Lemmas 3.6 and 3.7. Independent of the hopping matrix t and the chemical potential μ the Hamiltonian H will always be invariant under a global (i.e., all spins are equally transformed) **spin transformation** $\mathcal{W}_{\mathrm{s}}=\mathcal{W}_{\mathrm{s}}(w)$

$$\mathcal{W}_{\mathrm{s}}c^\dagger_{x,\sigma}\mathcal{W}_{\mathrm{s}}^\dagger:=\sum_{\sigma'}w_{\sigma',\sigma}c^\dagger_{x,\sigma'} \tag{3d.40}$$

for all $x\in\Lambda$, where $w\in U(2)$ is a unitary 2×2-matrix. Note that $\mathcal{W}_{\mathrm{s}}$ is a Bogoliubov transformation.

As always we shall be particularly interested in the spin *rotations*, i.e. transformations $\mathcal{W}_{\mathrm{s}}(w)$ corresponding to w in $SU(2)$. The full $U(2)$ group is generated by the $SU(2)$ subgroup together with the subgroup (isomorphic to $U(1)$) consisting of all $w_\theta=\begin{pmatrix} e^{i\theta} & \\ & e^{i\theta} \end{pmatrix}$, $0\leq\theta<2\pi$. The Bogoliubov transformation $\mathcal{W}_\theta:=\mathcal{W}_{\mathrm{s}}(w_\theta)$ is a global **phase change**, i.e.,

$$\mathcal{W}_\theta c^\dagger_{x,\sigma}\mathcal{W}_\theta^\dagger:=e^{i\theta}c^\dagger_{x,\sigma} \tag{3d.41}$$

for all $x\in\Lambda$. Spin rotations and phase changes (i.e., the full $U(2)$ group) exhaust the symmetries of the Hamiltonian H unless we assume more about the hopping matrix t.

The spin rotations are generated by the (quadratic) spin operators

$$\begin{aligned} \mathcal{S}_1=&\tfrac{1}{2}\sum_{x\in\Lambda}\left(c^\dagger_{x,\uparrow}c_{x,\downarrow}+c^\dagger_{x,\downarrow}c_{x,\uparrow}\right), \quad \mathcal{S}_2=\tfrac{1}{2i}\sum_{x\in\Lambda}\left(c^\dagger_{x,\uparrow}c_{x,\downarrow}-c^\dagger_{x,\downarrow}c_{x,\uparrow}\right), \\ \mathcal{S}_3=&\tfrac{1}{2}\sum_{x\in\Lambda}\left(c^\dagger_{x,\uparrow}c_{x,\uparrow}-c^\dagger_{x,\downarrow}c_{x,\downarrow}\right). \end{aligned}$$

The $U(1)$ phase change is generated by the number operator $\mathcal{N} = \sum_{x,\sigma} c^\dagger_{x,\sigma} c_{x,\sigma}$.

According to (2.a9) the Bogoliubov transformation $\mathcal{W}_{\mathrm{s}}(w)$ has its counterpart acting on $\mathcal{H} \oplus \mathcal{H}$ which we will denote by $W_{\mathrm{s}}(w)$ and in the special case of a phase change by W_θ. Indeed,

$$W_{\mathrm{s}}(w) = \begin{pmatrix} w & \\ & \overline{w} \end{pmatrix} \quad \text{and} \quad W_\theta = \begin{pmatrix} e^{i\theta} & & & \\ & e^{i\theta} & & \\ & & e^{-i\theta} & \\ & & & e^{-i\theta} \end{pmatrix}. \tag{3d.42}$$

From Lemma 3.1 it is easy to conclude that any Γ minimizing the energy functional (3.37b) corresponds to a HF ground state with total spin zero, i.e., a state with $\rho(\mathcal{S}_1^2 + \mathcal{S}_2^2 + \mathcal{S}_3^2) = 0$.

3.9 THEOREM (Zero total spin): *A 1-pdm Γ corresponds to an $SU(2)$ invariant HF state if and only if it has the form (3b.2). In particular, the HF ground states have total spin zero.*

Proof: The condition that a state be $SU(2)$ invariant is that Γ commutes with $W_s(w)$ for all $w \in SU(2)$. Recalling that the only 2×2 matrices commuting with all elements in $SU(2)$ are multiples of the identity matrix it follows easily that exactly the matrices of the form (3b.2) commute with all $W_s(w)$. It then follows that the HF ground states have total spin zero since they are pure states.■

The HF states are, however, not necessarily invariant under the $U(1)$ phase symmetries. If we use the unitary operator Y defined in (3b.11) we can write

$$YW_\theta Y^\dagger = \begin{pmatrix} W'_\theta & 0 \\ 0 & W'_\theta \end{pmatrix},$$

where

$$W'_\theta = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}. \tag{3d.43}$$

A 1-*pdm* Γ will therefore commute with W_θ if and only if the corresponding Γ' commutes with W'_θ. In case of the minimizing Γ'_0 it follows from (3b.31) (for positive temperature) or (3c.4) (for the zero temperature ground states) that Γ'_0 commutes with W'_θ if and only if the corresponding matrix-valued potential D_0 commutes with W'_θ. From (3b.24) and (3d.43) we find

$$W'_\theta D_x W'^\dagger_\theta = W'_\theta \begin{pmatrix} d(x) & \delta(x) \\ \overline{\delta(x)} & -d(x) \end{pmatrix} W'^\dagger_\theta = \begin{pmatrix} d(x) & e^{2i\theta}\delta(x) \\ e^{-2i\theta}\overline{\delta(x)} & -d(x) \end{pmatrix}. \tag{3d.44}$$

Thus D_0 commutes with W'_θ if and only if $\delta(x) = 0$, which not surprisingly is exactly the condition that the state is normal. Notice that (3d.44) agrees precisely with the characterization of the possible minimizers given in Lemma 3.6.

Note also that (3d.44) yields the same 1-*pdm* for $\theta + \pi (\mathrm{mod}\ 2\pi)$ as for θ, meaning that the representation of the group $U(1)$ by the minimizing states is not faithful. This reflects the fact, that generalized HF-states ρ obey the particular restriction $\rho(e_1 \ldots e_{2k+1}) = 0$, where e_i is either a c or a $c^\dagger$.

Now, let us consider the case in which t is bipartite and $\mu = 0$. Whether t is real or not the Hamiltonian H is invariant under the **particle-hole transformation**

$$\begin{aligned} \mathcal{W}_{\mathrm{ph}} \alpha c^\dagger_{x,\sigma} \mathcal{W}_{\mathrm{ph}} &:= (-1)^x \overline{\alpha} c_{x,\sigma}, \\ \mathcal{W}_{\mathrm{ph}} \alpha c_{x,\sigma} \mathcal{W}_{\mathrm{ph}} &:= (-1)^x \overline{\alpha} c^\dagger_{x,\sigma}, \end{aligned} \tag{3d.45}$$

where α is any complex number which we insert to indicate that $\mathcal{W}_{\rm ph}$ is antiunitary. In fact, for t non-real the particle-hole symmetry of the Hamiltonian cannot be unitarily realized. On $\mathcal{H}\oplus\mathcal{H}$, with the fixed basis $\{(x,\sigma)|x\in\Lambda,\sigma=\uparrow,\downarrow\}$ in $\mathcal{H}$, $\mathcal{W}_{\rm ph}$ corresponds to (the 4×4 operator) $W_{\rm ph}$, acting on operators as (A, B, C and D are here 2×2 operators)

$$W_{\rm ph}\begin{pmatrix} A & B \\ C & D\end{pmatrix} W_{\rm ph}^{-1} = (-1)^x \begin{pmatrix} \overline{D} & \overline{C} \\ \overline{B} & \overline{A}\end{pmatrix}(-1)^x. \tag{3d.46}$$

As for the $U(1)$ symmetry we would like to write $W_{\rm ph}$ in terms of a symmetry on $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$. This is only possible if we first compose it with a spin rotation which after all will leave our states invariant by Theorem 3.9. In fact, if $w=\begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}$ we have

$$YW_s(w)W_{\rm ph}Y^\dagger = (-1)^x\begin{pmatrix} W'_{\rm ph} & \\ & W'_{\rm ph}\end{pmatrix},$$

where $W'_{\rm ph}$ is the antiunitary map on $\mathcal{H}_\Lambda\oplus\mathcal{H}_\Lambda$ with matrix (in the standard basis) given by

$$W'_{\rm ph} = \begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}.$$

In order to understand the transformation property of a minimizing Γ'_0 it is again enough to consider the potential.

$$W'_{\rm ph}\begin{pmatrix} d & \delta \\ \overline{\delta} & -d\end{pmatrix} W'^{-1}_{\rm ph} = \begin{pmatrix} -d & -\delta \\ -\overline{\delta} & d\end{pmatrix} = -\begin{pmatrix} d & \delta \\ \overline{\delta} & -d\end{pmatrix} \tag{3d.47}$$

since $(-1)^x D(-1)^x = D$.

If t is not real we compare this with our result from Lemma 3.7. According to the condition on the minimizing D therein, we must have $\delta(x)=0$ for all $x\in\Lambda$. The minimizing D is, hence, of the form $D=\sum_x D_x\mathbf{1}_x$ or $D=\sum_x -D_x\mathbf{1}_x$ where

$$D_x = \begin{pmatrix} d(x) & \\ & -d(x)\end{pmatrix}. \tag{3d.48}$$

Thus, assuming that t is bipartite and non-real and $\mu=0$, the minimizing 1-*pdm* Γ has no pairs and corresponds to a normal state. It is unaffected by spin rotations and phase changes which means it has spin zero and fixed particle number. Only the particle-hole symmetry is broken due to the global change $d(x)\to -d(x)$ for all $x\in\Lambda$.

In case of a real, bipartite t at $\mu=0$ the symmetry group of the Hamiltonian is even larger. Let us introduce the Bogoliubov transformation $\mathcal{W}_{\rm bp}$ by

$$\begin{aligned} \mathcal{W}_{\rm bp}c^\dagger_{x\uparrow}\mathcal{W}^\dagger_{\rm bp} &= c^\dagger_{x\uparrow}, \\ \mathcal{W}_{\rm bp}c^\dagger_{x\downarrow}\mathcal{W}^\dagger_{\rm bp} &= (-1)^x c_{x\downarrow}. \end{aligned} \tag{3d.49}$$

The global **pseudo-spin rotation** $\mathcal{W}_{\rm ps}$ is given by

$$\mathcal{W}_{\rm ps}(w) = \mathcal{W}^\dagger_{\rm bp}\mathcal{W}_{\rm s}(w)\mathcal{W}_{\rm bp}, \tag{3d.50}$$

for any spin rotation $\mathcal{W}_{\rm s}(w)$, with $w \in SU(2)$. It leaves the Hamiltonian invariant in the real bipartite case at $\mu = 0$.

As in the spin case we could of course have considered the full group of $U(2)$ pseudo-spin transformations. The transformation $\mathcal{W}_{\rm ps}(w_\theta)$ corresponding to $w_\theta = \begin{pmatrix} e^{i\theta} & \\ & e^{i\theta} \end{pmatrix}$ is, however, equal to the spin rotation corresponding to $\widetilde{w}_\theta := \begin{pmatrix} e^{i\theta} & \\ & e^{-i\theta} \end{pmatrix}$, i.e. $\mathcal{W}_{\rm ps}(w_\theta) = \mathcal{W}_{\rm s}(\widetilde{w}_\theta)$. Conversely, the $U(1)$ group of phase change symmetries is really a subgroup of the $SU(2)$ pseudo-spin rotations. In fact, the pseudo-spin rotations are generated by the pseudo-spin operators

$$
\begin{aligned}
\widetilde{\mathcal{S}}_1 =& \tfrac{1}{2}\sum_{x\in\Lambda}(-1)^x\left(c^\dagger_{x,\uparrow}c^\dagger_{x,\downarrow} + c_{x,\downarrow}c_{x,\uparrow}\right), \quad \widetilde{\mathcal{S}}_2 = \tfrac{1}{2i}\sum_{x\in\Lambda}(-1)^x\left(c^\dagger_{x,\uparrow}c^\dagger_{x,\downarrow} - c_{x,\downarrow}c_{x,\uparrow}\right),\\
\widetilde{\mathcal{S}}_3 =& \tfrac{1}{2}\sum_{x\in\Lambda}\left(c^\dagger_{x,\uparrow}c_{x,\uparrow} - c_{x,\downarrow}c^\dagger_{x,\downarrow}\right) = \tfrac{1}{2}\mathcal{N} - \tfrac{1}{2}|\Lambda|\mathbf{1}.
\end{aligned}
$$

Notice that in terms of how they transform operators, i.e., $A \mapsto \mathcal{W}A\mathcal{W}^\dagger$ we cannot distinguish the unitaries

$$\exp(\tfrac{i}{2}\mathcal{N}\theta) \quad \text{and} \quad \exp(i\widetilde{\mathcal{S}}_3\theta).$$

We also point out that for real t the particle-hole symmetry may be unitarily realized as $\widetilde{\mathcal{W}}_{\rm ph} = \mathcal{W}_{\rm s}(w)\mathcal{W}^\dagger_{\rm bp}\mathcal{W}_{\rm s}(w^\dagger)\mathcal{W}_{\rm bp}$ with $w = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ and is, therefore, contained in the group of spin- and pseudo-spin rotations.

The unitary operator $W_{\rm ps}(w)$ on $\mathcal{H}\oplus\mathcal{H}$ corresponding to a $w \in SU(2)$ which we write as $w = \begin{pmatrix} w_{\uparrow\uparrow} & w_{\uparrow\downarrow} \\ -\overline{w}_{\uparrow\downarrow} & \overline{w}_{\uparrow\uparrow} \end{pmatrix}$ is given by

$$
W_{\rm ps}(w) = \begin{pmatrix} w_{\uparrow\uparrow} & & & (-1)^x w_{\uparrow\downarrow} \\ & w_{\uparrow\uparrow} & -(-1)^x w_{\uparrow\downarrow} & \\ & (-1)^x\overline{w}_{\uparrow\downarrow} & \overline{w}_{\uparrow\uparrow} & \\ -(-1)^x\overline{w}_{\uparrow\downarrow} & & & \overline{w}_{\uparrow\uparrow} \end{pmatrix}. \tag{3d.51}
$$

Thus, $YW_{\rm ps}(w)Y^\dagger = \begin{pmatrix} W'_{\rm ps}(w) & \\ & W'_{\rm ps}(w) \end{pmatrix}$, where

$$
W'_{\rm ps}(w) = \begin{pmatrix} w_{\uparrow\uparrow} & (-1)^x w_{\uparrow\downarrow} \\ -(-1)^x\overline{w}_{\uparrow\downarrow} & \overline{w}_{\uparrow\uparrow} \end{pmatrix}. \tag{3d.52}
$$

In other words, $W'_{\rm ps}(w)D_xW'_{\rm ps}(w)^\dagger$ is the transformation of the potential D_x. Now observe that if D_x fulfills (3d.19) then so does $W'_{\rm ps}(w)D_xW'_{\rm ps}(w)^\dagger$, indeed, starting from D with $\delta = 0$, (3d.19) simply states that all minimizers are of the form

$$W'_{\rm ps}(w)DW'_{\rm ps}(w)^\dagger \tag{3d.53}$$

with an arbitrary $SU(2)$-matrix w. Hence, for real, bipartite t at $\mu = 0$ the situation is as follows. Whenever δ is different from 0, the minimizing Γ does not correspond to a normal state and the particle number is broken. Likewise, the pseudo-spin rotation is a broken symmetry, as can be seen from (3d.53).

The complete tables to illustrate the broken symmetries can be found in Chapter V.

III.e SPATIAL UNIQUENESS OF MINIMIZERS

In the previous section we saw that if a minimizing potential D is nonvanishing there is a whole family of minimizers related by global gauge transformations of D. In fact, the phase of δ or the pseudo-spin must be aligned over the lattice and we can only allow global gauge transformations. The aim in this section is to prove that all degeneracies of the minimizing potentials D are caused by these gauge transformations. Since the HF ground and Gibbs states are uniquely determined by D it shows that the only degeneracies of these HF states are due to the symmetries discussed in the previous section.

More precisely, we shall show that if D_1 and D_2 are two minimizers for $\mathcal{R}_{\beta,\mu}$ then $D_1^2 = D_2^2$, i.e., $n_1 = n_2$, where as before $n_{1,2} = \sqrt{d_{1,2}^2 + |\delta_{1,2}|^2}$. We show this in the case where t is bipartite and $\mu = 0$. If t is not bipartite or $\mu \neq 0$ we also get $d_1 = d_2$ (see Lemma 3.11). The uniqueness statement in the bipartite case with $\mu = 0$ is an immediate consequence of the strict convexity we now prove.

3.10 LEMMA (Convexity of $\mathcal{R}_{\beta,0}$): *If t is bipartite (not necessarily real) and $\mu = 0$ then $\mathcal{R}_{\beta,0}\Big((-1)^x n, 0\Big)$, regarded as a functional of the function $\eta = n^2$ is convex. It is strictly convex at η if $\eta(x) \neq 0$ for all x*†.

Proof: We shall prove that if $n_0 = \sqrt{\lambda n_1^2 + (1-\lambda) n_2^2}$ for some $0 < \lambda < 1$ then

$$\mathcal{R}_{\beta,0}\Big((-1)^x n_0, 0\Big) \leq \lambda \mathcal{R}_{\beta,0}\Big((-1)^x n_1, 0\Big) + (1-\lambda)\mathcal{R}_{\beta,0}\Big((-1)^x n_2, 0\Big) \tag{3e.1}$$

with equality if and only if $n_1 = n_2 = n_0$. Since the term $\sum_x \mathrm{Tr}[D_x^2]$ is linear in n^2 we may ignore it here and we only need to consider the first term in (3d.2–3). Let D_j, $j = 0, 1, 2$ denote the potentials corresponding to $(d_j, \delta_j) = ((-1)^x n_j, 0)$, for $j = 0, 1, 2$.

To prove the strict convexity we assume $n_0(x) \neq 0$ (i.e., either $n_1(x) \neq 0$ or $n_2(x) \neq 0$) for all $x \in \Lambda$. If n_0 vanishes somewhere we still get convexity (but not strict) by a continuity argument. For both D_1 and D_2 we use (3d.24) with $B = U_x^{-1} n_0(x)^{-1}$ and we find

$$\ln \mathrm{Det}\Big[c^2 + (T - UD_j)^2\Big] \leq \ln \mathrm{Det}[A_*(c, D_j)] - 2 \ln \mathrm{Det}[B]. \tag{3e.2}$$

Since $D_j^2 = n_j^2 \mathbf{1}$ we get from the definition (3d.22) that $A_*(c, D_1) + A_*(c, D_2) = A_*(c, D_0)$. By strict concavity of $\ln \mathrm{Det}[\,\cdot\,]$ we obtain

$$\begin{aligned}\lambda \ln \mathrm{Det}\Big[c^2 + (T - UD_1)^2\Big] &+ (1-\lambda) \ln \mathrm{Det}\Big[c^2 + (T - UD_2)^2\Big] \\ &\leq \ln \mathrm{Det}\Big[A_*(c, D_0)\Big] - 2 \ln \mathrm{Det}[B] \\ &= \ln \mathrm{Det}\Big[c^2 + (T - UD_0)^2\Big],\end{aligned} \tag{3e.3}$$

† The convexity is, in fact, strict for all η, but this is more complicated to prove.

with equality if and only if $n_1 = n_2 = n_0$. The last equality in (3e.3) follows from $\{\widehat{T}, U\widehat{D}_0\} = 0$. Inserting (3e.3) into (3d.2-d3) gives (3e.1).■

If we do not assume bipartiteness and $\mu = 0$ the situation is somewhat more compicated. We have the following convexity result. Note that assuming $t - \mu$ not bipartite includes bipartite t with $\mu \neq 0$.

3.11 LEMMA (Convexity of $\mathcal{R}_{\beta,\mu}$): *If t is real $\mathcal{R}_{\beta,\mu}(d, \sqrt{n^2 - d^2})$, regarded as a functional of d and $\eta = n^2$ is convex, but not always strictly convex. If $t - \mu$ is not bipartite the functional $\mathcal{R}_{\beta,\mu}(d, \sqrt{n^2 - d^2})$ is minimized by unique functions d and n.*

Proof: We first prove the convexity. Note that $\mathcal{R}_{\beta,\mu}$ as a functional of the functions $\eta = n^2$ and d is defined on the convex set $\{(\eta, d) \mid |d|^2 \leq \eta\}$. Given d_j and n_j for $j = 1, 2$ satisfying $|d_j| \leq n_j$. Define $d_0 = \lambda d_1 + (1-\lambda) d_2$ and $n_0 = \sqrt{\lambda n_1^2 + (1-\lambda) n_2^2}$. Our aim is to prove that

$$\mathcal{R}_{\beta,\mu}\Big(d_0, \sqrt{n_0^2 - d_0^2}\Big) \leq \lambda \mathcal{R}_{\beta,\mu}\Big(d_1, \sqrt{n_1^2 - d_1^2}\Big) + (1-\lambda)\mathcal{R}_{\beta,\mu}\Big(d_2, \sqrt{n_2^2 - d_2^2}\Big). \tag{3e.4}$$

Let D_j for $j = 0, 1, 2$ correspond to $(d_j, \delta_j) = (d_j, \sqrt{n_j^2 - d_j^2})$. Since we can otherwise use a continuity argument we may assume that $\delta_0(x) = \sqrt{n_0(x)^2 - d_0(x)^2} \neq 0$ for all $x \in \Lambda$.

For both D_1 and D_2 we use (3d.12) with $B = U_x^{-1}|\delta_0(x)|^{-1} = U_x^{-1}\Big(n_0(x)^2 - d_0(x)^2\Big)^{-1/2}$. We obtain

$$\ln \mathrm{Det}\Big[c^2 + (T - UD_j)^2\Big] \leq \ln \mathrm{Det}\Big[A(c, D_j)\Big] - 2 \ln \mathrm{Det}[B], \tag{3e.5}$$

with equality if and only if $\{\widehat{T}_\mu, \widehat{G}_j\}$ vanishes. Using $A(c, D_1) + A(c, D_2) = A(c, D_0)$

$$\begin{aligned}\lambda \ln\mathrm{Det}\Big[c^2 + (T - UD_1)^2\Big] &+ (1-\lambda) \ln \mathrm{Det}\Big[c^2 + (T - UD_2)^2\Big] \\ &\leq \ln \mathrm{Det}\Big[A(c, D_0)\Big] - 2\ln \mathrm{Det}[B] = \ln \mathrm{Det}\Big[c^2 + (T - UD_0)^2\Big].\end{aligned} \tag{3e.6}$$

The last equality in (3e.6) holds because $\{\widehat{T}_\mu, \widehat{G}_0\}$ vanishes. The convexity in (3e.4) is an immediate consequence of (3e.6).

We have equality in (3e.6) if and only if $A(c, D_1) = A(c, D_2) = A(c, D_0)$, i.e.,

$$-\{\widehat{T}_\mu, \widehat{F}_1\} + \widehat{G}_1^2 + \widehat{F}_1^2 = -\{\widehat{T}_\mu, \widehat{F}_2\} + \widehat{G}_2^2 + \widehat{F}_2^2 = -\{\widehat{T}_\mu, \widehat{F}_0\} + \widehat{G}_0^2 + \widehat{F}_0^2. \tag{3e.7}$$

To show that $\mathcal{R}_{\beta,\mu}$ need not be strictly convex consider the case of bipartite t with $\mu \neq 0$. Let $d_1(x) = -U_x^{-1}\mu + (-1)^x c$ and $d_2(x) = -U_x^{-1}\mu - (-1)^x c$ for some $c > 0$ and let $\delta_1 = \delta_2 = 0$. If we take $\lambda = 1/2$ we find $d_0 = \frac{1}{2}d_1 + \frac{1}{2}d_2 = -U_x^{-1}\mu$ and $n_0^2 - d_0^2 = \frac{1}{2}d_1^2 + \frac{1}{2}d_2^2 - d_0^2 = c^2$. On the other hand by pseudo-spin invariance we see that strict convexity is violated:

$$\begin{aligned}\mathcal{R}_{\beta,\mu}(d_1, 0) = \mathcal{R}_{\beta,\mu}(d_2, 0) =& \mathcal{R}_{\beta,0}((-1)^x c, 0) + \sum_x U_x^{-1}\mu^2 \\ =& \mathcal{R}_{\beta,0}(0, c) + \sum_x U_x^{-1}\mu^2 = \mathcal{R}_{\beta,\mu}\left(d_0, \sqrt{n_0^2 - d_0^2}\right).\end{aligned}$$

Assume now that D_1 and D_2 are two minimizers for $\mathcal{R}_{\beta,\mu}$ and define D_0 as above with $\lambda = 1/2$. By convexity of $\mathcal{R}_{\beta,\mu}$ we conclude that D_0 is also a minimizer. Moreover, we know from Lemma 3.5ab that either $\delta_0(x) = 0$ for all x or $\delta_0(x) \neq 0$ for all x. If $\delta_0(x) = 0$ for all x we have

$$0 = n_0^2 - d_0^2 = \tfrac{1}{4}(d_1 - d_2)^2 + \tfrac{1}{2}\delta_1^2 + \tfrac{1}{2}\delta_2^2.$$

Hence $d_1 = d_2$ and $\delta_1 = \delta_2 = 0$ and thus $n_1 = n_2$.

If $\delta_0(x) \neq 0$ for all x, we know that (3e.7) is satisfied and that

$$\{\widehat{T}_\mu, \widehat{G}_j\} = 0 \tag{3e.8}$$

for $j = 0, 1, 2$. From the off-diagonal part of (3e.7) we conclude that for all $x \neq y$ in Λ with $t_{xy} \neq 0$ we have

$$\widehat{F}_{1x} + \widehat{F}_{1y} = \widehat{F}_{0x} + \widehat{F}_{0y}. \tag{3e.9}$$

Hence, $\widehat{F}_{1x} - \widehat{F}_{0x} = -(\widehat{F}_{1y} - \widehat{F}_{0y})$. If the off-diagonal part t' of t (i.e., $t'_{xy} = t_{xy} - t_{xx}\delta_{xy}$) is not bipartite we can find a path $z_1, z_2, \ldots, z_{2k} = z_1$ with an odd number of points such that $t'_{z_i z_{i+1}} \neq 0$. Therefore $F_{1z_1} = F_{0z_1}$ and by connectedness of t we then get $F_{1x} = F_{0x}$ for all x in Λ, i.e., $d_1 = d_0 = d_2$. It then easily follows from (3e.7) that also $n_1 = n_0 = n_2$.

We are left with the case where the off-diagonal part t' is bipartite. In this case we get from (3e.9):

$$|\delta_0(x)|^{-1}(d_1(x) - d_0(x)) = c(-1)^x \tag{3e.10}$$

for some constant c. We shall show now that if $c \neq 0$ then D_0 cannot be minimizing. By connectedness of t we see that (3e.8) implies that

$$\delta_1(x) = a_1\delta_0(x), \tag{3e.11}$$

where a_1 is a constant (recall that here $\delta_0(x)$ is positive) .

We turn to the diagonal part of (3e.7):

$$(t_{xx} - \mu - U_x d_1(x))^2 + U_x^2|\delta_1(x)|^2 = (t_{xx} - \mu - U_x d_0)^2 + U_x^2\delta_0(x)^2. \tag{3e.12}$$

If we insert (3e.10) and (3e.11) into (3e.12) we get

$$2c(-1)^x U_x^{-1}\delta_0(x)^{-1}(t_{xx} - \mu - U_x d_0(x)) + c^2 + |a_1|^2 = 1.$$

We therefore conclude that if $c \neq 0$ then

$$t_{xx} - \mu - U_x d_0(x) = (-1)^x U_x \delta_0(x) C, \tag{3e.13}$$

where C is a constant. We can restate this as

$$T_\mu - UD_0 = \begin{pmatrix} t' & \\ & -t' \end{pmatrix} - U_x\delta_0(x)\begin{pmatrix} (-1)^x C & 1 \\ 1 & -(-1)^x C \end{pmatrix}. \tag{3e.14}$$

We can choose a pseudo-spin rotation W as in (3d.52) such that

$$W\begin{pmatrix} (-1)^x C & 1 \\ 1 & -(-1)^x C \end{pmatrix}W^\dagger = \begin{pmatrix} & 1 + C^2 \\ 1 + C^2 & \end{pmatrix}. \tag{3e.15}$$

Since t' is assumed to be bipartite we see that the unitary operator

$$V = \sum_x (-1)^x \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \mathbf{1}_x$$

has the effect $VW(T_\mu - UD)W^\dagger V^\dagger = W(T_\mu - UD)W^\dagger$.

From (3b.31) and (3c.4) we see that if Γ' is the minimizer corresponding to D_0 then $\Gamma' = F_\beta((T_\mu - UD_0))$ where F_β is the function $F_\beta(\lambda) = [1+\exp(\beta\lambda/2)]^{-1}$ (for $\beta = \infty$ we have $F_\infty(\lambda) = \lim_{\beta\to\infty} F_\beta(\lambda) = \chi(\lambda)$). Hence $VW\Gamma' W^\dagger V^\dagger = W\Gamma' W^\dagger$. For the potential D_0 this implies that

$$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix} WD_0W^\dagger \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} = WD_0W^\dagger.$$

Since $WD_0W^\dagger$ is traceless we see in particular that the diagonal entries of $WD_0W^\dagger$ must be zero. If we write

$$D_{0x} = \delta_0(x) \begin{pmatrix} d_0(x)\delta_0(x)^{-1} & 1 \\ 1 & -d_0(x)\delta_0(x)^{-1} \end{pmatrix}$$

we see by comparison with (3e.15) that we must have $d_0(x)\delta_0(x)^{-1} = (-1)^x C$. It then follows from (3e.13) that $t_{xx} - \mu = 0$. Since we are in the case where t' is bipartite this implies that $t - \mu$ is bipartite contrary to our assumption in the lemma. ■

We can now state the main result of Chapter 3.

3.12 MAIN THEOREM (Characterization of HF states): *The HF Gibbs states or ground states are unique modulo global gauge transformations. More precisely, all HF Gibbs states at the same inverse temperature β or all HF ground states (i.e., the minimizers of the functionals (3b.23) and (3c.2) respectively) are related by global gauge transformations.*

Proof: By Theorems 3.3 and 3.4 there is a one to one correspondence between the HF states described by Γ' minimizing $-\mathcal{P}_{\beta,\mu}$ and the potentials D minimizing $\mathcal{R}_{\beta,\mu}$. The uniqueness of D modulo gauge transformations follows immediately from the results about $\mathcal{R}_{\beta,\mu}$; Lemmas 3.6–3.8 and Lemmas 3.10 and 3.11. ■

We remark that Theorem 3.12 allows us to characterize the HF Gibbs states by the global gauge and the inverse temperature. Indeed, the correspondence between β and the HF Gibbs state $\Gamma'(\beta, w)$ is continuous in β for every fixed global gauge w (w being a pseudo-spin rotation, or a phase change). In particular, this mapping is continuous at $\beta = \infty$ and, a posteriori, we could have spared the entire discussion of the zero temperature state by simply appealing to this continuity.

We shall see in Sect. III.g that if the temperature is high enough their maybe no symmetry breaking and hence the Gibbs state is unique. There is no degeneracy caused by gauge transformations. If however, the temperature is small it follows from Lemma 3.5 that there is symmetry breaking for any finite system. In the translation invariant case studied in Sect. III.g, the symmetry breaking phase transition persists in the thermodynamic limit.

III.f SPATIAL SYMMETRIES

In Sect. III.d we studied global gauge symmetries of the Hamiltonian. In the present section we shall address the question of spatial symmetries, i.e., symmetries of the lattice or, more precisely, of the t matrix and the coupling constants U_x.

As a special example, in the next section we shall explicitly determine the minimizing matrix-valued potential D when the lattice is translation invariant and the coupling constants U_x are independent of x.

By a **spatial symmetry** we understand an invertible transformation $\tau : \Lambda \mapsto \Lambda$ of the lattice Λ. We say that t is **magnetically invariant** under τ if there exists a map $\alpha_\tau : \Lambda \mapsto \mathbf{R}$ such that

$$t_{\tau(x)\tau(y)} = \exp[-i(\alpha_\tau(x) - \alpha_\tau(y))]t_{xy}.$$

Equivalently, if we realize t as an operator on $\mathcal{H}$ magnetic invariance means that t commutes with the unitary transformation $m(\tau)$ on $\mathcal{H}$ defined by

$$m(\tau)|x, \sigma\rangle = \exp(-i\alpha_\tau(x))|\tau(x), \sigma\rangle.$$

We need the phase factor α in order to treat non-real t. If t is real we may of course choose $\alpha_\tau = 0$. As an example consider a two-dimensional torus, i.e., a finite cube Λ in $\mathbf{Z}^2$ with periodic boundary conditions. The original (real) hopping matrix considered by Hubbard, Kanamori and Gutzwiller is invariant under pure translations ($m(\tau)$ with $\alpha_\tau = 0$) on the torus. Consider, however, the (complex) hopping matrix t which differs from the elements of the original matrix by the multiplication of complex phases and which correspond to having a fixed magnetic flux through each unit square. Then t is not invariant under pure translations but rather under the *magnetic* translations $m(\tau)$ which are compositions of translations and gauge transformations ($\alpha_\tau \neq 0$).

The family of all transformations τ for which t is magnetically invariant and the coupling constants satisfy $U_{\tau(x)} = U_x$ for all x in Λ naturally forms a group $\mathcal{G}$ which we call the **spatial symmetry group** (of t and U). Notice that $\tau \mapsto m(\tau)$ need not be a unitary representation of $\mathcal{G}$. In fact for the two-dimensional torus the translations commute while the magnetic translations do not. (If τ_1, τ_2 denote the translations of unit length along the first and second direction respectively we have $m(\tau_1)m(\tau_2) = \exp(i\phi)m(\tau_2)m(\tau_1)$, where ϕ is the flux through the unit squares.) We emphasize that the group $\mathcal{G}$ itself need not be abelian, it could be one of the crystallographic groups (e.g. if we study the Hubbard model on the lattice formed by the carbon atoms in the Buckminsterfullerene C_{60} molecule). We say that t is **translation invariant** if the spatial symmetry group $\mathcal{G}$ acts transitively on the lattice Λ, i.e., if for any two points $x, y \in \Lambda$ there is a τ in $\mathcal{G}$ such that $\tau(x) = y$. If t is bipartite (and connected) it is easy to see that each element τ of $\mathcal{G}$ must either map the A and B sublattices into themselves ($\tau(A) = A$ and $\tau(B) = B$) or map the A sublattice to the B sublattice ($\tau(A) = B$). It is clear that the latter type of transformations exist only if $|A| = |B|$.

Corresponding to $\tau \in \mathcal{G}$ we define a Bogoliubov transformation $\mathcal{W}_\tau$ on the Fock space $\mathcal{F}$ by

$$\mathcal{W}_\tau c^\dagger_{x,\sigma} \mathcal{W}^\dagger_\tau = \exp(-i\alpha_\tau(x))c^\dagger_{\tau(x),\sigma}.$$

The unitary matrix W_τ corresponding to $\mathcal{W}_\tau$ is

$$W_\tau = \begin{pmatrix} m(\tau) & \\ & \overline{m(\tau)} \end{pmatrix}.$$

If τ belongs to the spatial symmetry group then the Hubbard Hamiltonian is invariant under $\mathcal{W}_\tau$. We shall prove in the next lemma that if t is also non-bipartite then the HF Gibbs states are also invariant under $\mathcal{W}_\tau$. In the bipartite case the states are also invariant under transformations such that $\tau(A) = A$ and hence $\tau(B) = B$, they need, however, not be invariant under transformations such that $\tau(A) = B$.

3.13 THEOREM (Spatial invariance): *Let $\mathcal{G}$ be the group of spatial symmetries of t and U.*

(a) If t is bipartite (but not necessarily real) and $\mu = 0$ all minimizing potentials D for $\mathcal{R}_{\beta,0}$ satisfy that $n(x) = \sqrt{\frac{1}{2}\mathrm{Tr}[D_x^2]}$ is invariant under $\mathcal{G}$, i.e., $n(\tau(x)) = n(x)$ for all $\tau \in \mathcal{G}$. All minimizing Γ' for $-\mathcal{P}_{\beta,0}$ are invariant under W_τ unless τ maps the A sublattice to the B sublattice ($\tau(A) = B$). As a consequence the HF ground and Gibbs states are invariant under $\mathcal{W}_\tau$ unless $\tau(A) = B$.

(b) Assume t real and $t - \mu$ not bipartite Then the minimizers D for $\mathcal{R}_{\beta,\mu}$, Γ' for $-\mathcal{P}_{\beta,\mu}$ and the HF ground and Gibbs states are invariant under $\mathcal{G}$.

Proof: Part (a) follows from the strict convexity proved in Lemma 3.10 since it implies that n is unique and hence invariant. The second statement in part (a) is a consequence of Lemma 3.7. where all the possible minimizers D are described. In fact, the minimizers D are invariant under τ unless $\tau(A) = B$ because the 2×2-matrix valued function w_x defined in Lemma 3.7 is constant on the A sublattice and on the B sublattice.

Part (b) follows from Lemma 3.11 and Lemma 3.6 ■

III.g THE TRANSLATION INVARIANT CASE

In this section we shall explicitly determine the minimizing matrix-valued potential D under the additional assumption that the lattice is translational invariant, i.e., that the spatial isometry group G of t and U acts transitively. In particular this means that U is constant independent of x.

As shall be shown, there occurs a phase transition as the temperature varies about a critical value T_c, or β_c, respectively, provided $1 < \frac{U}{|\Lambda|}\mathrm{Tr}_{\mathcal{H}_\Lambda}[|t-\mu|^{-1}] < \infty$ holds and assuming that the spectrum of $t - \mu$ is symmetric about 0. More precisely, we will show that $D_x \equiv 0$, i.e. $n(x) = 0$ for all $x \in \Lambda$, if $\beta \leq \beta_c$ and $n(x)$ equal to a non-zero constant n_0 for all $x \in \Lambda$ in case of $\beta > \beta_c$.

Since, as we pointed out in section III.d, $n(x) = n_0 > 0$ goes along with having non-vanishing aligned pseudo-spins everywhere in Λ, this implies long range order which is off-diagonal in case that $\delta(x) \neq 0$ for all $x \in \Lambda$.

Secondly, due to the analytical dependence of the pressure on D, the transition from $n \equiv 0$ for $\beta \leq \beta_c$ to $n > 0$ for $\beta > \beta_c$ also indicates that the pressure is nonanalytic at β_c. Notice that in our model there is no thermodynamic limit $|\Lambda| \longrightarrow \infty$ required to yield a nonanalytic thermodynamic potential.

3.14 THEOREM (Pressure in translation invariant case): *If t (with as usual $t - \mu$ either bipartite or real) and U are translation invariant the pressure is*

$$\mathcal{P}(\beta,\mu) = -\min_{d^2 \leq \eta}\Big\{-2\beta^{-1}\mathrm{Tr}\left[\ln\cosh\tfrac{\beta}{2}\sqrt{(t-\mu)^2 - 2Ud(t-\mu) + U^2\eta}\right] + U\eta|\Lambda|\Big\} + (2\beta^{-1}\ln 2 + \mu)|\Lambda|, \tag{3g.1}$$

where the minimum is over real constants d and η. The minimium in (3g.1) occurs at unique values $d_0(\beta,\mu)$ and $\eta_0(\beta,\mu)$ satisfying

$$d_0(\beta,\mu)^2 \leq \eta_0(\beta,\mu) \leq \tfrac{1}{4}. \tag{3g.2}$$

If $t - \mu$ is bipartite then $d_0(\beta,\mu) = 0$.

Moreover, if D is any minimizer for $\mathcal{R}_{\beta,\mu}$ then for all x we have $n(x)^2 = \frac{1}{2}\mathrm{Tr}[D_x^2] = \eta$. If $t-\mu$ is not bipartite we also have that the upper diagonal element of D_x is $d(x) = d_0$ for all x.

Proof: Since $x \mapsto -\ln\cosh\sqrt{x}$ is strictly convex and since we are minimizing over the convex domain $\{d_0^2 \le \eta_0\}$ we conclude that the minimum occurs at unique values. This is just a special case of the more general statements in Lemmas 3.10 and 3.11.

If $t-\mu$ is bipartite it is unitarily equivalent to $-(t-\mu)$ it then follows from (3.113) that if d_0 and η_0 are minimizing values then so are $-d_0$ and η_0. By uniqueness we therefore have that $d_0 = 0$.

If $t-\mu$ is bipartite we may without loss of generality assume t bipartite and $\mu = 0$. It then follows from part (a) of Theorem 3.13 that all minimizers D of $\mathcal{R}_{\beta,\mu}$ satisfy that $n(x)^2 = \frac{1}{2}\mathrm{Tr}[D_x^2]$ is a constant η. We see from Lemma 3.7 that D_x is of a form such that $(T_\mu - UD)^2 = T^2 + U^2D^2$. Since the minimum in (3g.1) occurs for $d_0 = 0$ we see from (3b.30) that (3g.1) is indeed a correct formula for the pressure.

If $t-\mu$ is not bipartite but real and if the functions d and η define a minimizer for $\mathcal{R}_{\beta,\mu}$ (in the sense of Lemma 3.11) it follows from the uniqueness proved in Theorem 3.5bb that d and η are independent of x. It is then clear from (3b.30) that (3g.1) is correct and that the parameters $\eta = \eta_0$ and $d = d_0$ are the unique minimizers in (3g.1). ■

We now restrict to the case when $t-\mu$ is bipartite or more generally to the case where $t-\mu$ is unitarily equivalent to $-(t-\mu)$ and

$$1 < \frac{U}{|\Lambda|}\mathrm{Tr}[|t-\mu|^{-1}] \le \infty \tag{3g.3}$$

holds. Then a critical inverse temperature $0 < \beta_c < \infty$ is uniquely determined by

$$1 = \frac{U}{|\Lambda|}\mathrm{Tr}\left[|t-\mu|^{-1}\tanh\Big(\beta_c|t-\mu|\Big)\right], \tag{3g.4}$$

since the right side in (3g.4) is continuous and grows monotonically with β_c from 0 to $U|\Lambda|^{-1}\mathrm{Tr}[|t-\mu|^{-1}]$.

The following theorem establishes that β_c is, indeed, critical, provided the spectrum of $t-\mu$ is symmetric about 0 because, then, $d_0(\beta,\mu)$ always vanishes and the issue of determining the minimizer D simplifies. Notice that in the case where $d_0 = 0$, the gap around zero in the spectrum of $T_\mu - UD$ is at least $2U\eta_0^{1/2}$. If $t-\mu$ has a zero eigenvalue then $2U\eta_0^{1/2}$ is precisely the value of gap.

3.15 THEOREM (Gap equation): *Let t be real, translation invariant and $U_x = U > 0$ for all $x \in \Lambda$. Assume that $t-\mu$ and $\mu - t$ are unitarily equivalent as in the case of a bipartite lattice with $\mu = 0$. Let β_c be given by (3g.4) in case (3g.3) holds and $\beta_c := \infty$ otherwise. Then $\eta_0 = 0$ for $\beta \le \beta_c$. Moreover, $\eta_0(\beta,\mu)$ is a strict monotonically increasing function in $\beta_c < \beta$ given by the gap equation*

$$1 = \tfrac{1}{2}\frac{U}{|\Lambda|}\mathrm{Tr}\left[\Big((t-\mu)^2 + U^2\eta_0\Big)^{-1/2}\tanh\Big(\tfrac{\beta}{2}\sqrt{(t-\mu)^2+U^2\eta_0}\Big)\right], \tag{3g.5}$$

provided $\beta_c < \infty$.

Proof: Equation (3g.5) follows by setting the derivative with respect to η of the expression on the right side of (3g.1) equal to zero. Note that since $\tanh x < 1$ (3g.5) implies

$$1 \leq \tfrac{1}{2}\frac{|U|}{|\Lambda|}\mathrm{Tr}\Big[(t-\mu)^2 + U^2\eta_0\Big]^{-1/2} \leq \tfrac{1}{2}\eta_0^{-1/2},$$

in agreement with our previous condition $\eta_0 \leq \frac{1}{4}$.

The monotonicity of $\eta_0(\beta,\mu)$ in $\beta > \beta_c$ is straightforward from (3g.5). ■

On a translation invariant lattice we may represent $t-\mu$ by its eigenvalues $\varepsilon_{\mathbf{k}}$ for $\mathbf{k} \in BZ$, the Brillouin zone, whose volume we denote by $|BZ|$. In the thermodynamic limit, $|\Lambda| \to \infty$, the gap equation (3g.5) then takes the more familiar form

$$1 = \tfrac{1}{2}\frac{|U|}{|BZ|}\int_{BZ}\Big(\varepsilon_{\mathbf{k}}^2 + U^2\eta_0\Big)^{-1/2}\tanh\Big(\tfrac{\beta}{2}\sqrt{\varepsilon_{\mathbf{k}}^2 + U^2\eta_0}\Big)\,d\mathbf{k},$$

which is the BCS gap equation.

IV. THE GENERALIZED HF THEORY FOR THE HUBBARD MODEL WITH REPULSIVE INTERACTION

IV.a LINEARIZATION OF THE PRESSURE FUNCTIONAL

In this section the generalized HF theory will be applied to the Hubbard model with repulsive interaction. We continue to use the notation of Chapter III and consider the Hamiltonian

$$H_+ = \sum_{\substack{x,y\in\lambda\\ \sigma}} t_{xy}c_{x,\sigma}^\dagger c_{y,\sigma} + \sum_{x\in i} U_x\big(c_{x,\uparrow}^\dagger c_{x,\uparrow} - \tfrac{1}{2}\big)\big(c_{x,\downarrow}^\dagger c_{x,\downarrow} - \tfrac{1}{2}\big). \tag{4a.1}$$

which differs from H_- in (3a.1) in the reversed sign of the interaction, i.e., we again assume $U_x > 0$. A close look at the pair interaction reveals that $c_{x,\uparrow}^\dagger c_{x,\uparrow} c_{x,\downarrow}^\dagger c_{x,\downarrow} = c_{x,\uparrow}^\dagger c_{x,\downarrow}^\dagger c_{x,\downarrow} c_{x,\uparrow} \geq 0$. Thus the interaction (corresponding to the operator V in Chapter II) is repulsive and Theorem 2.11 applies. Hence, we may restrict our attention to 1-*pdm* of the form $\Gamma = \begin{pmatrix}\gamma & \\ & \mathbf{1}-\overline{\gamma}\end{pmatrix}$ and the energy expectation reduces to

$$\mathcal{E}(\Gamma) = \mathrm{Tr}[T_0'\gamma] + \sum_{x\in\Lambda} U_x\big\{[\gamma_\uparrow(x) - \tfrac{1}{2}][\gamma_\downarrow(x) - \tfrac{1}{2}] - |\gamma_*(x)|^2\big\}, \tag{4a.2}$$

where $\gamma_\sigma(x) := \langle x,\sigma|\gamma|x,\sigma\rangle$, $\gamma_*(x) := \langle x,\uparrow|\gamma|x,\downarrow\rangle$ and we denoted

$$T_\mu' := \begin{pmatrix} t-\mu & 0 \\ 0 & t-\mu\end{pmatrix} \tag{4a.3}$$

on $\mathcal{H}$. Obviously, $\mathcal{E}(\Gamma)$ depends on γ only and we will write $\mathcal{E}(\gamma) := \mathcal{E}(\Gamma)$. In fact, dealing merely with γ we will have to consider only operators on $\mathcal{H}$ rather than $\mathcal{H}\oplus\mathcal{H}$ throughout this chapter.

We denote $Q_x := \mathbf{1}_x Q \mathbf{1}_x$ for any operator Q on $\mathcal{H}$ where $\mathbf{1}_x$ is now the projection onto functions in $\mathcal{H}$ vanishing everywhere except at x.

Equipped with this notation we may write

$$\gamma_x = \begin{pmatrix} \gamma_\uparrow(x) & \overline{\gamma_*}(x) \\ \gamma_*(x) & \gamma_\downarrow(x) \end{pmatrix} \mathbf{1}_x \tag{4a.4}$$

and one easily verifies that

$$[\gamma_\uparrow(x) - \tfrac{1}{2}][\gamma_\downarrow(x) - \tfrac{1}{2}] - |\gamma_*(x)|^2 = \tfrac{1}{2}\left(\mathrm{Tr}[\gamma_x - \tfrac{1}{2}\mathbf{1}_x]\right)^2 - \tfrac{1}{2}\mathrm{Tr}\left[(\gamma_x - \tfrac{1}{2}\mathbf{1}_x)^2\right]. \tag{4a.5}$$

The entropy depends merely on γ, too, namely

$$\begin{aligned} S(\gamma) &= -\tfrac{1}{2}\mathrm{Tr}[\Gamma \ln \Gamma + (\mathbf{1} - \Gamma)\ln(\mathbf{1} - \Gamma)] \\ &= -\mathrm{Tr}[\gamma \ln \gamma + (\mathbf{1} - \gamma)\ln(\mathbf{1} - \gamma)], \end{aligned} \tag{4a.6}$$

and so does the pressure expectation

$$\begin{aligned} -\mathcal{P}_{\beta,\mu}(\gamma) =& \mathrm{Tr}[T'_\mu \gamma] + \tfrac{1}{2}\sum_x U_x \left(\mathrm{Tr}[\gamma_x] - 1\right)^2 - \tfrac{1}{2}\sum_x U_x \mathrm{Tr}\left[(\gamma_x - \tfrac{1}{2}\mathbf{1}_x)^2\right] \\ &+ \beta^{-1}\mathrm{Tr}[\gamma \ln \gamma + (\mathbf{1} - \gamma)\ln(\mathbf{1} - \gamma)], \end{aligned} \tag{4a.7}$$

where we again denoted $S(\gamma) := S(\Gamma)$ and $\mathcal{P}_{\beta,\mu}(\gamma) := \mathcal{P}_{\beta,\mu}(\Gamma)$. For the examination of the HF ground states we denote $\mathcal{P}_{\infty,\mu} := \lim_{\beta\to\infty} \mathcal{P}_{\beta,\mu} = \mathcal{E} - \mu N$. Let us introduce an auxiliary functional

$$\begin{aligned} -\widehat{\mathcal{P}}_{\beta,\mu}(\gamma) =& \mathrm{Tr}[T'_\mu \gamma] - \tfrac{1}{2}\sum_x U_x \mathrm{Tr}\left[(\gamma_x - \tfrac{1}{2}\rho(x)\mathbf{1}_x)^2\right] \\ &+ \beta^{-1}\mathrm{Tr}[\gamma \ln \gamma + (\mathbf{1} - \gamma)\ln(\mathbf{1} - \gamma)], \end{aligned} \tag{4a.8}$$

denoting $\rho(x) := \mathrm{Tr}[\gamma_x]$. Of course, we write $\widehat{\mathcal{P}}_{\infty,\mu} := \lim_{\beta\to\infty} \widehat{\mathcal{P}}_{\beta,\mu}$. Notice the formal similarity between (4a.8) and (3b.23). Replacing T_μ by T'_μ and Γ' by γ in (3b.23) we arrive at (4a.8) excpet that $\rho(x)$ is missing (and that there is an extra unimportant term $-\mu|\Lambda|$ in (3b.23)). The reason $\rho(x)$ is missing in (3b.23) is that $\mathrm{Tr}[\Gamma'_x] = 1$ is a consequence of the form (3b.13). This is the crucial formal difference bewteen the attractive and repulsive cases. We claim that

$$-\mathcal{P}_{\beta,\mu}(\gamma) = -\widehat{\mathcal{P}}_{\beta,\mu}(\gamma) + \tfrac{1}{4}\sum_x U_x[\rho(x) - 1]^2. \tag{4a.9}$$

Indeed, since $\gamma_x - \frac{1}{2}\rho(x)\mathbf{1}_x$ has zero trace,

$$\begin{aligned} -\mathcal{P}_{\beta,\mu}(\gamma) + \widehat{\mathcal{P}}_{\beta,\mu}(\gamma) &= \tfrac{1}{2}\sum_x U_x \Big\{[\rho(x) - 1]^2 - \mathrm{Tr}\left[(\gamma_x - \tfrac{1}{2}\mathbf{1}_x)^2\right] + \mathrm{Tr}\left[(\gamma_x - \tfrac{1}{2}\rho(x)\mathbf{1}_x)^2\right]\Big\} \\ &= \tfrac{1}{2}\sum_x U_x \Big\{[\rho(x) - 1]^2 - \mathrm{Tr}\left[\tfrac{1}{2}[\rho(x) - 1]^2 \mathbf{1}_x\right]\Big\} \\ &= \tfrac{1}{4}\sum_x U_x [\rho(x) - 1]^2. \end{aligned} \tag{4a.10}$$

Equation (4a.9) is an important observation. With our machinery developed in Chapter III we can only determine the minimizers for $-\widehat{\mathcal{P}}_{\beta,\mu}$ rather than $-\mathcal{P}_{\beta,\mu}$. This substitution is justified only if we can show that a 1-*pdm* γ minimizing $-\widehat{\mathcal{P}}_{\beta,\mu}$ also minimizes $-\mathcal{P}_{\beta,\mu}$. We succeed in doing so *only* in case of bipartite hopping matrices t with chemical potential $\mu = 0$. In fact, in this case we will prove that

$$\rho(x) = \mathrm{Tr}[\gamma_x] = \sum_\sigma \langle x,\sigma|\gamma|x,\sigma\rangle = 1 \tag{4a.11}$$

for all lattice points $x \in \Lambda$. We shall refer to (4a.11) as the **constant density lemma** because of its similarity to the main theorem in [LLM]. Equation (4a.11) establishes the formal analogy between the attractive and repulsive cases.

We start with the analysis of $-\widehat{\mathcal{P}}_{\beta,\mu}$ and its minimizer. We will denote

$$-\widehat{\mathcal{P}}(\beta,\mu) := \min_{0\le\gamma\le\mathbf{1}} -\widehat{\mathcal{P}}_{\beta,\mu}(\gamma) \tag{4a.12}$$

for positive or infinite β. In analogy with (3b.25) we first observe that

$$-\mathrm{Tr}\left[(\gamma_x - \tfrac{1}{2}\rho(x)\mathbf{1}_x)^2\right] = \min_{d,\delta}\left\{-2\mathrm{Tr}[D_x\gamma_x] + \mathrm{Tr}[D_x^2]\right\}, \tag{4a.13}$$

where $D_x := \begin{pmatrix} d(x) & \overline{\delta}(x) \\ \delta(x) & -d(x)\end{pmatrix}$. Because of (4a.13) the proof of the following lemma is a line-by-line copy of the one for Theorems 3.3 and 3.4.

4.1 LEMMA: *For all $0 < \beta \le \infty$ and all μ we can write the auxiliary functional $\widehat{\mathcal{P}}(\beta,\mu)$ as the following variation over the functions d and δ.*

$$-\widehat{\mathcal{P}}(\beta,\mu) = \min_{d,\delta}\mathcal{R}_{\beta,\mu}(d,\delta) - 2\beta^{-1}|\Lambda|\ln 2, \tag{4a.14}$$

where

$$\mathcal{R}_{\beta,\mu}(d,\delta) := \mathcal{R}_{\beta,\mu}(D) := -\,\beta^{-1}\mathrm{Tr}[\ln\cosh\tfrac{\beta}{2}(T'_\mu - UD)] + \tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2], \tag{4a.15a}$$

and

$$\mathcal{R}_{\infty,\mu}(d,\delta) := \mathcal{R}_{\infty,\mu}(D) := -\,\tfrac{1}{2}\mathrm{Tr}|T'_\mu - UD| + \tfrac{1}{2}\sum_x U_x\mathrm{Tr}[D_x^2]. \tag{4.a15b}$$

If a potential D minimizes $\mathcal{R}_{\beta,\mu}$ then the operator

$$\gamma = \left(\mathbf{1} + \exp\Big[\beta(T'_\mu - UD)\Big]\right)^{-1}, \ \textit{for } \beta<\infty \quad \textit{or} \quad \gamma = \chi(T'_\mu - UD), \ \textit{for } \beta = \infty \tag{4a.16}$$

minimizes the auxiliary functional $-\widehat{\mathcal{P}}_{\beta,\mu}$ and satisfies the consistency equation

$$\gamma_x = \left(D_x + \tfrac{1}{2}\mathrm{Tr}[\gamma_x]\right)\mathbf{1}_x. \tag{4a.17}$$

Conversely, if γ is a minimizer for $-\widehat{\mathcal{P}}_{\beta,\mu}$ then the potential D defined by (4a.17) minimizes $\mathcal{R}_{\beta,\mu}$ and satisfies (4a.16).

As in the attractive case the minimum in (4a.14) occurs for functions d and δ satisfying $d(x)^2 + |\delta(x)|^2 \le \frac{1}{4}$ for all $x \in \Lambda$.

We prove an analog of Lemma 3.5 by merely replacing T_μ by T'_μ in the proof of that lemma.

4.2 LEMMA (Gap estimate): *Let D be a minimizing matrix-valued potential for $\mathcal{R}_{\beta,\mu}$ or $\mathcal{R}_{\infty,\mu}$ and denote the eigenvalues of $T_\mu - UD$ by $e_1, e_2, \ldots, e_{2|\Lambda|}$. Then, for any $j = 1, 2, \ldots, 2|\Lambda|$, we have*

$$|e_j| \geq \tfrac{1}{4} U_{\min} |\Lambda|^{-1} - \beta^{-1} 2 \ln 2 \qquad \text{or} \qquad |e_j| \geq \tfrac{1}{4} U_{\min} |\Lambda|^{-1}, \tag{4a.18}$$

respectively, where $U_{\min} := \min_{x \in \Lambda} \{U_x\}$.

Lemma 4.1 allows us to concentrate now on the determination of the functions d and δ that yield a minimizer D for $\mathcal{R}_{\beta,\mu}$ or $\mathcal{R}_{\infty,\mu}$ respectively. Note that $\mathcal{R}_{\beta,\mu}$ in the repulsive case differs from $\mathcal{R}_{\beta,\mu}$ in the attractive case only by the replacement of T_μ by T'_μ.

IV.b CONSTANT DENSITY LEMMA FOR BIPARTITE LATTICES AT HALF-FILLING

In this section we will assume that the hopping matrix t is bipartite (possibly non-real) and the chemical potential μ equals zero. It will turn out that this choice of t and μ allows us to conclude that $\mathrm{Tr}[\gamma] = |\Lambda| = \frac{1}{2} \dim \mathcal{H}$ which is the reason for calling this case *half-filling.*

4.3 LEMMA (Antiferromagnetic spin alignment): *Let t be bipartite (but not necessarily real) and $\mu = 0$. Then*

$$\mathcal{R}_{\beta,\mu}(d, \delta) \geq \mathcal{R}_{\beta,\mu}\left((-1)^x \sqrt{d^2 + |\delta|^2}, 0 \right). \tag{4b.1}$$

If $n(x) := \sqrt{d^2(x) + |\delta(x)|^2} > 0$ for all $x \in \Lambda$ equality holds in (4b.1) if and only if for all $x \in \lambda$

$$\begin{pmatrix} d(x) & \delta(x) \\ \overline{\delta}(x) & -d(x) \end{pmatrix} = (-1)^x n(x) w \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} w^\dagger \tag{4b.2}$$

for some unitary 2×2-matrix w independent of $x \in \Lambda$.

The proof of Lemma 4.3 is in complete anology to the proof of Lemma 3.7. We merely have to replace T_0 by T'_0. Notice that (4b.2) results from

$$t_{xy} \left[\frac{d(x)}{n(x)} - \frac{d(y)}{n(y)} \right] = 0, \qquad t_{xy} \left[\frac{\delta(x)}{n(x)} - \frac{\delta(y)}{n(y)} \right] = 0, \tag{4b.3}$$

which replaces the conditions (3d.25a) and (3d.25b) in the proof of Lemma 3.7. Note that (4b.2) shows that the potential D has the staggered order characteristic of antiferromagnetism. The form (4b.2) is exactly what we need to prove the constant density lemma.

4.4 LEMMA (Constant density): *Let t be bipartite (but not necessarily real) and $\mu = 0$. Define γ by*

$$\gamma := \left(\mathbf{1} + \exp[\beta(T'_0 - UD)] \right)^{-1}, \tag{4b.4}$$

where D_x is subject to condition (4b.2) for some unitary 2×2-matrix w. Then

$$\mathrm{Tr}[\gamma_x] = \sum_\sigma \langle x, \sigma | \gamma | x, \sigma \rangle = 1. \tag{4b.5}$$

In particular, $\mathrm{Tr}[\gamma] = \sum_x \mathrm{Tr}[\gamma_x] = |\Lambda|$.

Proof: We want to show that

$$0 = \sum_\sigma \langle x, \sigma | \tfrac{1}{2} - \gamma | x, \sigma \rangle = \tfrac{1}{2} \sum_\sigma \langle x, \sigma | \tanh \tfrac{1}{2} \beta (T'_0 - UD) | x, \sigma \rangle. \tag{4b.6}$$

We define a unitary transformation

$$V_w := w \begin{pmatrix} 0 & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} w^\dagger (-1)^x. \tag{4b.7}$$

One easily checks that

$$V_w (T_0' - UD) V_w^\dagger = -(T_0' - UD). \tag{4b.8}$$

Thus,

$$\begin{aligned} \sum_\sigma \langle x, \sigma | \tanh \tfrac{1}{2}\beta(T_0' - UD) | x, \sigma\rangle &= \sum_\sigma \langle x, \sigma | V_w \left[\tanh \tfrac{1}{2}\beta(T_0' - UD)\right] V_w^\dagger | x, \sigma\rangle \\ &= -\sum_\sigma \langle x, \sigma | \tanh \tfrac{1}{2}\beta(T_0' - UD) | x, \sigma\rangle, \end{aligned} \tag{4b.9}$$

which is equivalent to (4b.6). ■

Now we are in a position to determine the actual pressure.

4.5 MAIN THEOREM (Ground state and positive temperature pressure): *Let t be bipartite and $\mu = 0$. Then for all $0 < \beta \le \infty$*

$$-\mathcal{P}(\beta, 0) = -\widehat{\mathcal{P}}(\beta, 0) = \min_{d,\delta} \mathcal{R}_{\beta,0}(d, \delta) - 2\beta^{-1}|\Lambda| \ln 2. \tag{4b.10}$$

If a potential D minimizes $\mathcal{R}_{\beta,0}$ for $0 < \beta \le \infty$ then γ defined in (4a.16) is a HF Gibbs state ($\beta < \infty$) or ground state ($\beta = \infty$). This γ satisfies the consistency equation

$$\gamma_x = (D_x + \tfrac{1}{2})\mathbf{1}_x. \tag{4b.11}$$

The function $n(x) = \sqrt{d(x)^2 + |\delta(x)|^2}$ corresponding to a minimizer D is unique and vanishes either everywhere or else nowhere. The potential D_x must be of the form (4b.2) for some unitary matrix w. As a consequence, the HF Gibbs states and ground states are unique modulo gauge transformations.

Proof: The right side of (4b.10) is clearly a lower bound to $-\mathcal{P}(\beta, 0)$ since $-\mathcal{P}_{\beta,0}(\gamma) \ge -\widehat{\mathcal{P}}_{\beta,0}(\gamma)$ for any $0 \le \gamma \le \mathbf{1}$. On the other hand by Lemma 4.3 the minimum on the right side of (4b.10) can be attained by a potential D satisfying (4b.2) (e.g. with w equal to the identity matrix). We then have a minimizer γ for $\widehat{\mathcal{P}}$ defined in terms of D by (4a.16) (with $\mu = 0$). Note that because of the gap estimate we know that $\chi(T_0' - UD) = \lim_{\beta\to\infty}(\mathbf{1} + \exp[\beta(T_0' - UD)])^{-1}$. It therefore follows for both finite and infinite β that γ satisfies the constant density relation (4b.5). Thus by (4a.9),

$$-\mathcal{P}(\beta, 0) \le -\mathcal{P}_{\beta,0}(\gamma) = -\widehat{\mathcal{P}}_{\beta,0}(\gamma). \tag{4b.12}$$

This conludes the proof that γ is a HF Gibbs or ground state. The remaining part of the heorem follows by an analysis identical to the one leading to Lemma 3.8, Lemma 3.10 and Theorem 3.12 (part of the conclusion is that $\mathcal{R}_{\beta,0}((-1)^x n, 0)$ is convex as a function of $\eta = n^2$ and strictly convex at its minimum). ■

Finally, we mention that a result on spatial symmetry analogous to Theorem 3.13 (with the same proof) holds in the repulsive case.

4.6 THEOREM (Spatial invariance): *Assume t is bipartite (not necessarily real) and $\mu = 0$ and let $\mathcal{G}$ be the group of spatial symmetries of t and U. For any minimizer (d, δ) of $\mathcal{R}_{\beta,0}$ we* *have that the function* $n(x) = \sqrt{d(x)^2 + |\delta(x)|^2}$ *is invariant under* $\mathcal{G}$. *The HF ground and Gibbs states are invariant under* $\mathcal{W}_\tau$ *for* $\tau \in \mathcal{G}$ *unless* $\tau(A) = B$.

IV.c PARTICLE-HOLE SYMMETRY

In the special case of a *real* bipartite hopping matrix t at half-filling $\mu = 0$ there is a more elegant way of deducing Theorems 4.5 and 4.6 from Theorems 3.2, 3.5 and 3.8 by means of a **partial particle-hole transformation** only on the $\uparrow$-spins. More precisely, we define the Bogoliubov transformation $\mathcal{W}_{ph,\uparrow}$ by

$$\begin{aligned} \mathcal{W}_{ph,\uparrow} c^\dagger_{x,\uparrow} \mathcal{W}^\dagger_{ph,\uparrow} &= (-1)^x c_{x,\uparrow}, \\ \mathcal{W}_{ph,\uparrow} c^\dagger_{x,\downarrow} \mathcal{W}^\dagger_{ph,\uparrow} &= c^\dagger_{x,\downarrow}. \end{aligned} \tag{4c.1}$$

Then

$$\begin{aligned} \mathcal{W}_{ph,\uparrow} H_+ \mathcal{W}^\dagger_{ph,\uparrow} =& \sum_{x,y} t_{xy} (-c_{x,\uparrow} c^\dagger_{y,\uparrow} + c^\dagger_{x,\downarrow} c_{y,\downarrow}) + \sum_x U_x (c_{x,\uparrow} c^\dagger_{x,\uparrow} - \tfrac{1}{2})(c^\dagger_{x,\downarrow} c_{x,\downarrow} - \tfrac{1}{2}) \\ =& \sum_{x,y} (\bar{t}_{xy} c^\dagger_{x,\uparrow} c_{y,\uparrow} + t_{xy} c^\dagger_{x,\downarrow} c_{y,\downarrow}) - \sum_x t_{xx} \\ & - \sum_x U_x (c^\dagger_{x,\uparrow} c_{x,\uparrow} - \tfrac{1}{2})(c^\dagger_{x,\downarrow} c_{x,\downarrow} - \tfrac{1}{2}) \\ =& H_-, \end{aligned} \tag{4c.2}$$

using $t_{xy} = \bar{t}_{xy} = t_{yx}$, the canonical anticommutation relations and $\sum_x t_{xx} = 0$. Since the Bogoliubov transformation leave the set of quasi-free states invariant, it immediately follows that

$$\begin{aligned} E^{\mathrm{HF}}(H_-) =& \inf \{\rho(H_-) \mid \rho \text{ is quasi-free } \} \\ =& \inf \left\{\rho_{\mathcal{W}_{ph,\uparrow}}(H_-) \mid \rho \text{ is quasi-free } \right\} \\ =& \inf \{\rho(H_+) \mid \rho \text{ is quasi-free } \} \\ =& E^{\mathrm{HF}}(H_+) \end{aligned} \tag{4c.3}$$

and a similar equality holds for the pressure at finite temperatures. Thus, there is clearly a one-to-one correspondence between the 1-*pdm* Γ_+ minimizing the generalized HF pressure functional for H_+ and the 1-*pdm* Γ_- minimizing the generalized HF pressure functional for H_- via

$$\Gamma_+ = \mathcal{W}_{ph,\uparrow} \Gamma_- \mathcal{W}^\dagger_{ph,\uparrow}. \tag{4c.4}$$

Note that if t is *not* real the attractive and repulsive cases are *not* unitarily equivalent. In fact, it follows from Theorems 3.5 and 4.5 that in the attractive case there may be no more than two minimizers, while in the repulsive case there is a continuous family of minimizers related by spin $SU(2)$ transformations.

IV.d FERROMAGNETISM AT INFINITE REPULSION

In the preceding sections we found that for bipartite lattices at *half-filling*, $N = |\Lambda|$, the minimizing 1-*pdm* always has *antiferromagnetic order*, i.e., the sign of d on the A-sublattice is always opposite to the sign on the B-sublattice. On the other hand Nagaoka's Theorem states that the true ground state (which happens to be the free particle HF state) for $N = |\Lambda| - 1$ has maximal spin $S = N/2$, provided one takes $U = \infty$ (see [NY], [TD], [TH]). In our language this would mean that the ground state γ would satisfy (after an $SU(2)$ rotation) $\gamma_\downarrow(x) = 0$. Setting $U = \infty$ mathematically, means, projecting out the vectors with doubly occupied sites from the full Fock space.

In the context of the generalized HF approximation one can also make sense of $U = \infty$ and we will derive an analog of Nagaoka's Theorem for the HF minimizer. The analogy goes too far, however, because as we will prove for any $1 \le N \le |\Lambda| - 1$ the HF ground state γ_0 will be fully spin polarized. In contrast, for the true Hubbard model this does not hold, i.e. for $N = |\Lambda| - 2$ (see [DW], [DFR], [TB],[SA]) or for $N \le 0.51|\Lambda|$ [SKA], the ground state does not have $S = N/2$.

Let us start by defining what is meant by infinite repulsion in the context of generalized HF theory. Recall from (4.2) that the energy functional for positive coupling $U_x = U > 0$ becomes

$$\begin{aligned}\mathcal{E}(\gamma) =& \mathrm{Tr}[T_0'\gamma] + U \sum_{x\in\Lambda} \left\{[\gamma_\uparrow(x) - \tfrac{1}{2}][\gamma_\downarrow(x) - \tfrac{1}{2}] - |\gamma_*(x)|^2\right\} \\ =& \mathrm{Tr}[T_0'\gamma] + U \sum_{x\in\Lambda} \left[\gamma_\uparrow(x)\gamma_\downarrow(x) - |\gamma_*(x)|^2\right] + \tfrac{1}{4}U|\Lambda| - \tfrac{1}{2}U\mathrm{Tr}[\gamma]. \end{aligned} \tag{4d.1}$$

We consider the particle number $N = \mathrm{Tr}[\gamma]$ fixed. The last two terms in (4d.1) are therefore constants that we may ignore when determining the minimizing γ. The limit $U \to \infty$ yields the constraint

$$\gamma_\uparrow(x)\gamma_\downarrow(x) - |\gamma_*(x)|^2 = 0 \tag{4d.2}$$

for any $x \in \Lambda$. More precisely, if we define the Hartree-Fock energy of N electrons by

$$E_U^{\mathrm{HF}}(N) := \inf\left\{\mathcal{E}(\gamma) + \tfrac{1}{2}UN - \tfrac{1}{4}U|\Lambda| \;\middle|\; 0 \le \gamma \le \mathbf{1},\ \mathrm{Tr}[\gamma] = N\right\} \tag{4d.3}$$

then $\lim_{U\to\infty} E_U^{\mathrm{HF}}(N) = E_{U=\infty}^{\mathrm{HF}}(N)$ where

$$E_{U=\infty}^{\mathrm{HF}}(N) := \inf\left\{\mathrm{Tr}[T_0'\gamma] \;\middle|\; 0 \le \gamma \le \mathbf{1},\ \mathrm{Tr}[\gamma] = N, \gamma \text{ fulfills (4d.2) }\right\}. \tag{4d.4}$$

We remark that $N \le |\Lambda|$ is automatic in (4d.4) because the constraint (4d.2) is equivalent to $\mathrm{Det}[\gamma_x] = 0$, which together with $0 \le \gamma \le \mathbf{1}$ implies that $\mathrm{Tr}[\gamma_x] \le 1$ and hence $N = \sum_x \mathrm{Tr}[\gamma_x] \le |\Lambda|$.

4.7 THEOREM (Ferromagnetism at infinite U): *Let $e_1 \le e_2 \le \ldots \le e_{|\Lambda|}$ denote the eigenvalues of t. Then*

$$E_{U=\infty}^{\mathrm{HF}}(N) = \sum_{i=1}^{N} e_i. \tag{4d.5}$$

A family of minimizing γ for the variation in (4d.4) corresponds to the ferromagnetically saturated states i.e., is given by

$$\gamma = w \begin{pmatrix} P_N & \\ & 0 \end{pmatrix} w^\dagger, \tag{4d.6}$$

where w is any $SU(2)$ matrix and P_N is the spectral projection onto the eigenvectors with eigenvalues $e_1, e_2, \ldots, e_N$.

Proof: It is clear that $E^{\rm HF}_{U=\infty}(N) \le \sum_{i=1}^{N} e_i$. Because any matrix of the form (4d.6) is admissible for the variation in (4d.4). On the other hand given any γ satisfying (4d.2), $0 \le \gamma \le \mathbf{1}$ and $\mathrm{Tr}[\gamma] = N$. We can write

$$\gamma = \sum_i |\varphi_i\rangle\langle\varphi_i| = \sum_i |f_i \oplus g_i\rangle\langle f_i \oplus g_i|, \tag{4d.7}$$

where $\langle\varphi_i|\varphi_j\rangle \le \delta_{ij}$ for all i,j. On the right side of (4d.7) we regarded $\mathcal{H}$ as $\mathcal{H}_\uparrow \oplus \mathcal{H}_\downarrow$, and we denoted $f_i(x) := \varphi_i(x,\uparrow)$ and $g_i(x) := \varphi_i(x,\downarrow)$. Now, define on $\mathcal{H}_\Lambda$

$$\widetilde{\gamma}_\uparrow := \sum_i |f_i\rangle\langle f_i| + |g_i\rangle\langle g_i|, \tag{4d.8}$$

such that $\widetilde{\gamma} := \begin{pmatrix} \widetilde{\gamma}_\uparrow & \\ & 0 \end{pmatrix}$ is completely spin-up polarized. The 1-*pdm* $\widetilde{\gamma}$ naturally fulfills (4d.2). Our goal is to show that $\widetilde{\gamma}_\uparrow \le \mathbf{1}$ and hence $\widetilde{\gamma} \le \mathbf{1}$ since this, together with $0 \le \widetilde{\gamma}$ and $\mathrm{Tr}[\widetilde{\gamma}] = N$ implies (4d.5) because

$$\mathrm{Tr}[T_0'\gamma] = \mathrm{Tr}\,[T_0'\widetilde{\gamma}] = \mathrm{Tr}[t\widetilde{\gamma}_\uparrow] \ge \sum_{i=1}^{N} e_i. \tag{4d.9}$$

In order to demonstrate $\widetilde{\gamma}_\uparrow \le \mathbf{1}$ we need to take a closer look at the constraint (4d.2) first. We may rewrite (4d.2) as

$$\left(\sum_i |f_i(x)|^2\right)\left(\sum_i |g_i(x)|^2\right) - \left|\sum_i \overline{f_i(x)} g_i(x)\right|^2 = 0 \tag{4d.10}$$

for all $x \in \Lambda$. Let us denote

$$\Lambda_0 := \{x \in \Lambda \mid f_1(x) = f_2(x) = \cdots = f_N(x) = 0\}. \tag{4d.11}$$

On Λ_0 (4d.10) holds trivially, but on the complement it yields the existence of a complex number $\alpha(x)$ such that

$$g_1(x) = \alpha(x) f_1(x),\ g_2(x) = \alpha(x) f_2(x),\ \ldots, g_N(x) = \alpha(x) f_N(x) \tag{4d.12}$$

for any $x \in \Lambda \setminus \Lambda_0$ by Schwarz' "equality". We define a *normal* operator A, $AA^\dagger = A^\dagger A$ on $\mathcal{H}_\Lambda$ by

$$A := \sum_{x \in \Lambda\setminus\Lambda_0} \alpha(x) |x\rangle\langle x|, \tag{4d.13}$$

and denote the projection onto Λ_0 by $B := \sum_{x\in\Lambda_0} |x\rangle\langle x|$. Hence, we may express (4d.12) as $g_i = Af_i + Bg_i$. By means of A and B we can write

$$\begin{aligned}\delta_{ij} \ge \langle\varphi_i|\varphi_j\rangle = \langle f_i|f_j\rangle + \langle g_i|g_j\rangle &= \langle f_i|(\mathbf{1} + A^\dagger A) f_j\rangle + \langle g_i|Bg_j\rangle \\ &= \langle f_i|(\mathbf{1} + AA^\dagger) f_j\rangle + \langle g_i|Bg_j\rangle.\end{aligned} \tag{4d.14}$$

We define $F_i := |f_i\rangle\langle f_i|$, $G_i := |g_i\rangle\langle g_i|$, $R_i := B|g_i\rangle\langle f_i|$. Now, $\widetilde{\gamma}_\uparrow \leq \mathbf{1}$ and, therefore, (4d.5) are direct consequences of the inequality

$$\widetilde{\gamma}_\uparrow - \widetilde{\gamma}_\uparrow^2 \geq \left(\sum_i [A, F_i] + R_i\right)\left(\sum_i [A, F_i]^\dagger + R_i^\dagger\right) + \left(\sum_i R_i^\dagger\right)\left(\sum_i R_i\right). \tag{4d.15}$$

The inequality (4d.15) follows from (4d.14), $\widetilde{\gamma}_\uparrow = \sum_i F_i + G_i$, and $AA^\dagger = A^\dagger A$ since

$$\begin{aligned}
F_iF_j =& |f_i\rangle\langle f_i|f_j\rangle\langle f_j| \leq |f_i\rangle\Big(\delta_{ij} - \langle f_i|A^\dagger A|f_j\rangle - \langle g_i B g_j\rangle\Big)\langle f_j| \\
=& \delta_{ij}F_i - F_iA^\dagger AF_j - R_i^\dagger R_j, = \delta_{ij}F_i - F_iAA^\dagger F_j - R_i^\dagger R_j, \\
G_iG_j =& |g_i\rangle\langle g_i|g_j\rangle\langle g_j| \leq |g_i\rangle\Big(\delta_{ij} - \langle f_i|f_j\rangle\Big)\langle g_j| \\
=& \delta_{ij}G_i - AF_iF_jA^\dagger - R_iF_jA^\dagger - AF_iR_j^\dagger - R_iR_j^\dagger, \qquad (4d.16) \\
F_iG_j =& F_iAF_jA^\dagger + F_iAR_j^\dagger. \qquad \blacksquare
\end{aligned}$$

The previous theorem does not tell us when the ferromagnetically saturated states are the *only* HF ground states. The proof only gives the following criterion, which, unfortunately may be very difficult to verify. Assume that $e_N < e_{N+1}$ which ensures the uniqueness of P_N. The criterion for uniqueness of the ferromagnetically states given by 1-*pdm* of the form (4d.6) is that the spectral projection P_N be connected in the sense that any two points $x, y \in \Lambda$ can be connected by a path $x = x_0, x_1, \ldots, x_n = y$ for which $\langle x_i|P_N|x_{i+1}\rangle \neq 0$. To prove this criterion suppose that γ in (4d.4) is a minimizer, i.e.,

$$\mathrm{Tr}[T_0'\gamma] = \mathrm{Tr}_\Lambda[t\widetilde{\gamma}_\uparrow] = \sum_{i=1}^N e_i, \tag{4d.17}$$

where $\widetilde{\gamma}_\uparrow$ is defined as in (4d.7). Hence, $\widetilde{\gamma}_\uparrow = P_N = \widetilde{\gamma}_\uparrow^2$ and (4d.15) implies

$$\sum_i R_i = 0, \quad \left[A, \sum_i F_i\right] = 0, \tag{4d.18}$$

which, in turn, gives us

$$\begin{aligned}
P_N = \widetilde{\gamma}_\uparrow = \sum_i F_i + G_i =& \sum_i F_i + AF_iA^\dagger + AR_i + R_i^\dagger A^\dagger + BG_iB \\
=& \sum_i F_i + AF_iA^\dagger + BG_iB. \qquad (4d.19)
\end{aligned}$$

The right side of (4d.19) is not connected between Λ_0 and $\Lambda \setminus \Lambda_0$ unless $\Lambda_0 = \emptyset$ or $\Lambda_0 = \Lambda$. The case $\Lambda_0 = \Lambda$ simply means that γ is completely spin-down polarized, in accordance with (4d.6). Conversely assuming $\Lambda_0 = \emptyset$, we observe that (4d.19) also implies $[A, P_N] = 0$ and obtain

$$[\alpha(x) - \alpha(y)]\,\langle x|P_N|y\rangle = 0 \tag{4d.20}$$

for all $x, y \in \Lambda \setminus \Lambda_0 = \Lambda$. But P_N was assumed to be connected and, therefore, $\alpha(x)$ =const for all $x \in \Lambda$. In other words, $f_i = \alpha g_i$ for all i which implies (4d.6).

V. SUMMARY OF HF THEORY OF THE HUBBARD MODEL

V.a INTRODUCTION

Our aim here is to give some perspective to the results in Sects. III and IV by summarizing them—with special emphasis on symmetries and their breaking. The first task is to define **symmetry breaking**. We start with a Hamiltonian H that, in many cases, is invariant under some symmetry group, G, each element of which is represented by a unitary operator on our Hilbert (Fock) space of dimension $4^{|\Lambda|}$. The representation of the group G might be a ray representation, as in the case of "magnetic translations". The unitary operator corresponding to an element $w \in G$ will be denoted by $W(w)$ on the one-particle space $\mathcal{H} \oplus \mathcal{H}$ and by $\mathcal{W}(w)$ on the Fock space $\mathcal{F}$. Since the only unitaries that transform HF states into HF states are Bogoliubov transformations, we restrict our attention to groups consisting of such transformations. This restriction is not really a cause for disappointment because all the symmetry groups that are usually considered, such as rotations in real space, rotations in spin space, translations, etc. are, in fact, represented by Bogoliubov unitaries. The reason is simply that most symmetry groups in physics are defined by their action on one particle and are then extended to $N > 1$ particles by tensoring. This is exactly what number conserving Bogoliubov transformations do.

We shall take the point of view *that a state breaks a symmetry if the state is not invariant under the action of the corresponding symmetry group.* This is formalized as follows.

5.1 DEFINITION (Broken or unbroken symmetry): *Let G be a group represented by unitaries as described above. Let ρ be a state on the operators on Fock space $\mathcal{F}$ corresponding to the Hilbert space $\mathcal{H}$. We say that the G symmetry is* **unbroken** *in the state ρ if, for each $w \in G$, ρ is invariant under the Bogoliubov transformation $\mathcal{W}(w)$, i.e., $\rho\left(\mathcal{W}(w)A\mathcal{W}(w)^\dagger\right) = \rho(A)$. If the state is not invariant for all $w \in G$ we say that the G symmetry is* **broken** *in the state ρ.*

We are particularly interested in HF ground states or finite temperature Gibbs states for a Hamiltonian H invariant under the action of some group G, i.e., $\mathcal{W}(w)H\mathcal{W}(w)^\dagger = H$ for all $w \in G$. The interesting question is then whether or not the G symmetry is broken in these states.

The contrast between the usual theory and the HF theory should be kept in mind. While the original Schrödinger equation $H\psi = E\psi$ defines a linear theory, the HF theory that approximates it is intrinsically a **nonlinear, one-particle theory**. Linear combinations of HF wave functions (which are Bogoliubov transforms of the zero-particle vacuum) are **not** HF wave functions. On the level of **states** (either pure states, $A \mapsto \langle\psi|A|\psi\rangle$, or Gibbs states), the HF states do *not* form convex sets. Usually, if ρ_1 and ρ_2 are states (either ground states of some Hamiltonian H or Gibbs states of H at some temperature T—in the thermodynamic limit there can be more than one) then $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ is an admissible state (ground or Gibbs). As discussed in the introduction this is not true for HF states because ρ is not usually a HF state when ρ_1 and ρ_2 are. In the usual theory we can ask for the extremal states (i.e. those states that are not convex combinations of other states at the same temperature) and ask about their properties with respect to symmetry operations. An example to keep in mind here is the Heisenberg Hamiltonian, for which there is a magnetized ground state. By taking a convex combination of all ground states one can construct a ground state that is $SU(2)$ invariant, but this state is not extremal in the set of ground states. From this example we learn that in the usual theory symmetry breaking should be sought only with extremal states—which correspond to pure phases.

The HF states, on the other hand, do not form convex sets and therefore we cannot talk about extremal states. We regard each HF state, heuristically, as playing the role of an extremal state. Indeed, in the usual theory symmetry breaking in a finite system is infrequent; typically it is necessary to pass to the thermodynamic limit in order to see it. In contrast, if symmetry breaking occurs in HF theory, it is usually manifest for the finite system. The following discussion refers to either the ground state or to positive temperature states. It is to be understood that the symmetry breaking displayed in our three tables may not actually occur. In particular, they will usually not occur if the temperature is high enough.

V.b SYMMETRIES OF THE HUBBARD HAMILTONIAN

To begin our summary of symmetry breaking in the HF theory of the Hubbard model we first list the symmetries of the Hubbard Hamiltonian. There are two types of possible symmetries of H, global gauge symmetries and spatial symmetries. The spatial symmetries of H depend on the spatial symmetries of t and U as explained in Sect. III.f. The gauge symmetries depend on the presence or absence of the following three properties: Bipartiteness of t, reality of t, and $\mu = 0$. Whether the gauge symmetries are broken may depend on the sign of the interaction.

(i) Spatial symmetries: In Section III.f, Theorem 3.13, we found that the spatial symmetries (if any are present) are broken only for a bipartite t and then only when $\mu = 0$. Each spatial symmetry either maps A to A and B to B or maps A to B and B to A. Even for bipartite t and $\mu = 0$, the A to A symmetries are never broken. It is only the transformations τ in the spatial symmetry group which take the A sublattice into the B sublattice, i.e., $\tau(A) = B$ (hence of course $\tau(B) = A$) that are broken. In fact, in this case we must require that the two sublattices A and B have the same number of points ($|A| = |B|$). Whenever we refer to a broken spatial symmetry in the tables below, we always mean that it is only the symmetry of maps from A to B that is broken. (Note that there can be several maps from A to B, but by modding out by maps from A to A we are left with one map from A to B.)

For the very special case of a *real* bipartite t, $\mu = 0$ and attractive interaction there are states which do not even break the A to B symmetry. Indeed, according to (3d.19), there are states for which $d(x) = 0$ and $\delta(x)$ is constant on the whole lattice. These states are completely translation invariant.

The gauge symmetries of the Hubbard Hamiltonian that we shall consider are the following:

(ii) Spin $SU(2)$: The action of $SU(2)$ on the Fock space was defined in (3d.40). It is the Bogoliubov transform corresponding to a global spin rotation on the one-particle space $\mathcal{H}$. Every Hubbard Hamiltonian is invariant under this transformation.

(iii) Phase $U(1)$: The action of $U(1)$ is given by the Bogoliubov transformation (3d.41). Again, every Hubbard Hamiltonian is invariant under this $U(1)$ symmetry. A generator of the $U(1)$ transformation (3d.41) on Fock space is, in fact, the number operator $\mathcal{N}$. Thus, $U(1)$ invariance of a state implies particle conservation, but not necessarily a definite particle number. (See the remark after Theorem 2.3.) A normal state is precisely a state where the $U(1)$ symmetry is unbroken.

(iv) Pseudo-spin $SU(2)$: If we are in the real, bipartite case and $\mu = 0$ we have a very large symmetry group. In fact the spin $SU(2)$ symmetry is supplemented by the pseudo-spin $SU(2)$ symmetry defined in (3d.50).

Although the pseudo-spin $SU(2)$ commutes with the spin $SU(2)$, the pseudo-spin is not completely independent of the spin. More precisely, the full symmetry group generated by the spin $SU(2)$ and pseudo-spin $SU(2)$ transformations is not isomorphic to the group $SU(2) \times SU(2)$. The full symmetry group is $SO(4)$, see [YZ]. This is so because for the particular matrix $w = -\mathbf{1}$

in $SU(2)$, the spin transformation (i.e., the Bogoliubov transformation $\mathcal{W}$ on Fock space) corresponding to $(w,\mathbf{1}) \in SU(2)\times SU(2)$ is identical to the pseudo-spin transformation corresponding to $(\mathbf{1},w)\in SU(2)\times SU(2)$. This easily follows from (3d.51) with $w=-\mathbf{1}$ since the Bogoliubov transformation $\mathcal{W}_{\mathrm{s}}(w)$ commutes with the transformation $\mathcal{W}_{\mathrm{bp}}$. This also corresponds with the observation that the representations we obtain for the two spins are either both integer or both half-integer. For our purposes it is more useful, however, to treat the spin and pseudo-spin transformations independently. Indeed, there will be cases where the pseudo-spin $SU(2)$ is a broken symmetry but the spin $SU(2)$ is not and vice versa. Merely saying that the $SO(4)$ symmetry is broken would convey much less information. Likewise the $U(1)$ phase symmetry is just a subgroup of the pseudo-spin symmetry; the Bogoliubov transforamtion $\mathcal{W}_\theta$ in (3d.41) is equal to the pseudo-spin transformation $\mathcal{W}_{\mathrm{ps}}$ corresponding to $w=\begin{pmatrix} e^{i\theta} & 0\\ 0 & e^{-i\theta}\end{pmatrix}$ in $SU(2)$. We therefore emphasize in Table 2 in the case of broken pseudo-spin (t real and bipartite, positive interaction and $\mu=0$), that not only is the pseudo-spin broken but there even exist HF ground states or Gibbs states for which the subgroup $U(1)$ is broken. While the pseudo-spin is always broken in this case, there are states for which $U(1)$ is unbroken, i.e., there exist **normal** ground states and Gibbs states.

(v) Particle-hole $\mathbf{Z}_2$: The large symmetry group consisting of the spin $SU(2)$ and pseudo-spin $SU(2)$ required reality, bipartiteness and half-filling. If, however, we give up the condition of reality we saw in Section III.d that the particle-hole symmetry survives as the antiunitary transformation given in (3d.45).

In case that we have a real t we shall of course not distinguish the unitary and antiunitary particle hole transformations as different symmetries. In this case, breaking of pseudo-spin or of spin symmetry may or may not imply breaking of particle-hole symmetry (See table 2). According to (3d.47) (with an extra complex conjugation, because we are in the real t case) the $\mathbf{Z}_2$ symmetry is unbroken if and only if

$$\begin{pmatrix} d(x) & \delta(x)\\ \overline{\delta(x)} & -d(x)\end{pmatrix} = -\begin{pmatrix} d(x) & \overline{\delta(x)}\\ \delta(x) & -d(x)\end{pmatrix}, \tag{5b.1}$$

i.e., $d(x)=0$ and $\delta(x)$ is purely imaginary.

Notice that in the case where the pseudo-spin is a broken symmetry (t real bipartite, attractive interaction and $\mu=0$) the $U(1)$ symmetry must be broken when $\mathbf{Z}_2$ is unbroken and conversely $\mathbf{Z}_2$ must be broken when $U(1)$ is unbroken. Thus, there are two normal states in this case, related by a particle-hole transformation, and there is one state (which cannot be a normal state) that is invariant under the particle-hole transformation.

Note that the spatial A–B symmetry (if exists) is broken if and only if the $\mathbf{Z}_2$ particle hole symmetry is broken. Although, these are different symmetries, in the sense that they act as different transformations on the Fock space, they are identical when restricted to the HF ground states and Gibbs states.

The following diagram illustrates the relationships among the four gauge symetries: The particle-hole $\mathbf{Z}_2$ is a combination of spin and pseudo-spin, while the phase $U(1)$ is really a subgroup of the pseudo-spin $SU(2)$.

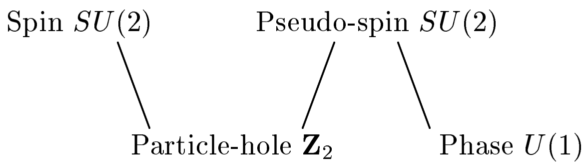

TABLE NO. 1 Non-Real t

	Symmetries of H	*Broken Symmetries*	*Spatial invariance*
Non-bipartite and/or $\mu \neq 0$	Spin $SU(2)$, $U(1)$	No results except for $U = \infty$, where spin $SU(2)$ is broken but $U(1)$ and spatial invariance are not.	
Bipartite $\mu = 0$ Attractive interaction*	Spin $SU(2)$, $U(1)$, $\mathbf{Z}_2$	$\mathbf{Z}_2$	A-B symmetry broken
Bipartite $\mu = 0$ Repulsive interaction*	Spin $SU(2)$, $U(1)$, $\mathbf{Z}_2$	Spin $SU(2)$, $\mathbf{Z}_2$	A-B symmetry broken

* Notice that even though we are in the bipartite case and $\mu = 0$, the attractive and repulsive interaction Hamiltonians are not unitarily equivalent when t is not real

TABLE NO. 2 Real Bipartite t

	Symmetries of H	*Broken Symmetries*	*Spatial invariance*
$\mu \neq 0$ Attractive interaction	Spin $SU(2)$, $U(1)$	$U(1)$	Not broken
$\mu = 0$ Attractive interaction*	Spin $SU(2)$, Pseudo spin $SU(2)$	Pseudo-spin $SU(2)$ (in particular $\mathbf{Z}_2$ and $U(1)$ can be broken)	A-B symmetry can be broken
$\mu \neq 0$ Repulsive interaction	Spin $SU(2)$, $U(1)$	No results except for $U = \infty$, where spin $SU(2)$ is broken but $U(1)$ and spatial invariance are not.	
$\mu = 0$ Repulsive interaction*	Spin $SU(2)$, Pseudo-spin $SU(2)$	Spin $SU(2)$ (in particular $\mathbf{Z}_2$ is broken)	A-B symmetry broken

* For real, bipartite t and $\mu = 0$ the Hamiltonians with attractive and repulsive interactions **are** unitarily equivalent. Because of the $(-1)^x$, a spatial symmetry between the A and B sublattices will not commute with this unitary transformation; hence Table 2 fails to be the same for the repulsive and attractive cases.

TABLE NO. 3 Real, Non-Bipartite t			
	Symmetries of H	*Broken Symmetries*	*Spatial invariance*
Attractive interaction Any μ	Spin $SU(2)$, $U(1)$	$U(1)$	Not broken
Repulsive interaction Any μ	Spin $SU(2)$, $U(1)$	No results except for $U=\infty$, where spin $SU(2)$ is broken but $U(1)$ and spatial invariance are not.	

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