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Density Functional Approach to Quantum Lattice Systems

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For quantum lattice systems, we consider the problem of characterizing the set of single-particle densities, ρ, which come from the ground-state eigenspace of some N-particle Hamiltonian of the form $H_0 + \sum_{i=1}^{N} v(x_i)$, where H_0 is a fixed, bounded operator representing the kinetic and interaction energies. We show that the conditions on ρ are that it be strictly positive, properly normalized, and consistent with the Pauli principle. Our results are valid for both finite and infinite lattices and for either bosons or fermions. The Coulomb interaction may be included in H_0 if the lattice dimension is $\geqslant 2$. We also characterize those single-particle densities which come from the Gibbs states of such Hamiltonians at finite temperature. In addition to the conditions stated above, ρ must satisfy a finite entropy condition.

KEY WORDS: Density functionals; Hohenberg–Kohn theory; V-representability; inverse problem.

1. INTRODUCTION

In 1964 Hohenberg and Kohn[(1)] suggested a novel approach (now referred to as HK theory) to the problem of finding the ground-state energy of a multiparticle Hamiltonian of the form

$$\begin{aligned} H &= -\sum_{j=1}^{N} \Delta_j + \sum_{j<k} u(x_j - x_k) + \sum_{j=1}^{N} v(x_j) \\ &\equiv H_0 + V \end{aligned} \tag{1.1}$$

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where N is the number of particles, $v(x)$ is a real-valued multiplication operator, and H_0 denotes the first two sums in (1.1). Traditionally, u is the Coulomb interaction, but many other interactions, including N-body rather that two-body interactions, can be used without significantly affecting the theory provided that the interaction is *fixed.*

The basic HK uniqueness theorem[(1)] states that if $v_1(x) \neq v_2(x) + \text{const}$, then the corresponding densities,[6] ρ_i, coming from the ground-state wave functions are also unequal, i.e., $\rho_1(x) \neq \rho_2(x)$. The HK uniqueness theorem implies that there is a one-to-one map $\mathscr{R}: v \to \rho$, between a suitable set of potentials and a corresponding set of densities. Therefore, physical quantities such as the ground-state energy, $\mathscr{E}$, can in principle be considered via $\mathscr{R}^{-1}(\rho)$ as functionals of the density. Despite the obvious impracticality of finding an explicit form for such functionals, HK theory has been widely used as the basis for approximation schemes and computations. (Most applications are based on the Kohn–Sham equations.[(2)] For a brief review see Ref. 3; for additional applications see Ref. 4.) A minimal condition for putting these variational schemes on a firm foundation is to restrict the variation to those ρ in $\text{range}(\mathscr{R}) = \text{domain}(\mathscr{E})$. The problem of characterizing the range of $\mathscr{R}$ is often referred to as the "V-representability" or "inverse" problem, and consists of finding conditions on ρ which guarantee that there is a single-particle potential $v(x)$ such that ρ comes from the ground state of $H_0 + V$.

The analogous problem for classical finite-temperature systems has also received attention (see, e.g., Ref. 5). For both the canonical and grand canonical distributions, sufficient conditions for V-representability have been obtained by Chayes, Chayes, and Lieb.[(6)] In the case of H-stable grand canonical systems, both necessary and sufficient conditions have been obtained.[(7)]

In this paper, we consider quantum lattice systems. For these systems, $-\Delta_j$, which represents the kinetic energy of particle j, denotes the finite difference Laplacian or "hopping" operator. We show that every density which is strictly positive, properly normalized, and consistent with the Pauli principle[7] comes from the ground-state eigenspace of $H_0 + V$ for some suitable potential. We also consider the generalization of HK theory to finite temperature and show that if, in addition to the above conditions, ρ satisfies a finite entropy condition, then ρ comes from the Gibbs equilibrium state of a unique Hamiltonian of the form (1.1). Our results are valid for both finite and infinite lattices, for either bosons or fermions, and for any fixed,

[6] By density, we always mean a single-particle density as defined in (1.3) or (1.6).

[7] In the case of fermions, the Pauli principle ensures that the density at any lattice site is smaller than the number of spin states. Saturation is not permitted for finite potentials [see discussion following equation (2.8)].

bounded interaction. It should be noted that this mild restriction on the interaction includes the electron gas, since the lattice Coulomb interaction is bounded in dimensions $\geqslant 2$. These results are discussed in Sections 2 and 3. For finite lattices, some partial and related results were obtained by Epstein and Rosenthal,[8] Kohn,[9] Englisch and Englisch,[10] and Katriel, Appellof, and Davidson.[24][8]

Although we are primarily concerned in this paper with proving sufficient conditions on ρ, as we discuss in Section 4, our conditions are also necessary, except possibly for fermions at zero temperature.

In order to place our results in perspective, we wish to summarize what is known about quantum continuous systems, which were the systems originally studied by Hohenberg and Kohn. Before doing so, it will be useful to introduce some notation. The single-particle reduced density matrix, γ, coming from the N-particle wave function Ψ is given by the kernel

$$\gamma(w, w') = \int \Psi(w, w_2,..., w_N)\, \bar{\Psi}(w', w_2,..., w_N)\, dw_2 \cdots dw_N \tag{1.2}$$

where $w_i = (x_i, \sigma_i)$ denotes both the space, x_i, and spin, σ_i, coordinates of the ith particle. When Ψ and γ are related by (1.2) we write $\Psi \mapsto \gamma$. The single-particle density, $\rho(x)$, is the function

$$\begin{aligned}\rho(x) &= N \sum_\sigma \gamma(w, w)\\ &= N \sum_{\sigma_1} |\Psi((x, \sigma_1), w_2,..., w_N)|^2\, dw_2 \cdots dw_N\end{aligned} \tag{1.3}$$

We write $\Psi \mapsto \rho$ and $\gamma \mapsto \rho$. If Γ is an N-particle density matrix, i.e.,

$$\Gamma(W, W') = \sum_k \alpha_k \Psi_k(W)\, \bar{\Psi}_k(W') \tag{1.4}$$

where $W = (w_1,..., w_N)$, $\alpha_k \geqslant 0$, and $\sum_k \alpha_k = 1$, then one can define the corresponding single-particle entities as

$$\gamma = \sum_k \alpha_k \gamma_k \tag{1.5}$$

and

$$\rho = \sum_k \alpha_k \rho_k \tag{1.6}$$

where $\Psi_k \mapsto \gamma_k \mapsto \rho_k$. Again we write $\Gamma \mapsto \gamma$ and $\Gamma \mapsto \rho$.

[8] In the case of *finite* lattices, a proof of Theorem 2.1 for bosons was given by Englisch and Englisch in Ref. 10. After submitting this manuscript, we learned that Englisch and Englisch have also obtained an independent proof of Theorem 2.1 for fermions on a *finite* lattice.[25] In both cases, the techniques used are quite different from those presented here.

The problem of characterizing the range of $\mathscr{R}$ was originally posed as follows: Under what conditions on candidate densities, ρ, is there a single-particle potential, v, such that $H_0 + V$ $[V = \sum_i v(x_i)]$ has a ground-state eigenfunction Ψ_0 satisfying $\Psi_0 \mapsto \rho$? Certain conditions are obvious:

(a) $\int \rho = N$.

(b) $\rho(x) \geqslant 0$.

In order to ensure that the kinetic energy of Ψ is finite whenever $\Psi \mapsto \rho$, it turns out[11] that the additional restriction

(c) $\int |\nabla \sqrt{\rho}|^2 < \infty$

should also be imposed. Conditions (a) and (c) are sometimes combined as[9] $\sqrt{\rho} \in H^1$, since one can always adjust the normalization.

For the purposes of V-representability one often considers a strengthened form of condition (b), namely $\rho(x) > 0$. While this condition may exclude some V-representable densities, there is a large class of potentials for which the corresponding densities are strictly positive. This follows from unique continuation theorems[12] and also from the results of Hoffmann-Ostenhof, Hoffmann-Ostenhof, and Simon[13] on the nodes of wave functions and, in the case of bosons, from Perron-Fröbenius type theorems.[12] It should be noted that naive prescriptions for relaxing the restriction $\rho(x) > 0$ [e.g., set $v(x) = \infty$ whenever $\rho(x) = 0$] can lead to serious difficulties.

In curious contrast to the quantum lattice case, the Pauli principle does not place any restrictions on range($\mathscr{R}$) for continuous systems. The reason is that one can always construct many single-particle density matices, γ, such that $\gamma \mapsto \rho$ and γ satisfies the Pauli principle.

These considerations suggest that one define

$$\mathscr{P} = \left\{ \rho \;\middle|\; \sqrt{\rho} \in H^1, \rho > 0, \int \rho = N \right\} \tag{1.7}$$

and ask whether every ρ in $\mathscr{P}$ comes from the ground-state eigenfunction of some potential v. That this is false was demonstrated by means of counterexamples constructed by Lieb[11] and Levy.[14] They consider a system of N fermions for which the ground state of $H_0 + V$ has degeneracy l. Let $\Gamma = P_0/l$, where P_0 projects onto the ground-state eigenspace of $H_0 + V$, and let ρ be the density of Γ, i.e., $\Gamma \mapsto \rho$. Lieb proved that it is possible to choose v so that $\Psi_j \not\mapsto \rho$ for any Ψ_j in the ground-state eigenspace of v or of any other potential.

Although HK theory was originally formulated for potentials with nondegenerate ground states, it has since been realized that it can be easily

[9] $H^1 = \{f \mid \int |f|^2 < \infty, \int |\nabla f|^2 < \infty\}$.

extended to include the possibility of degenerate ground states. For example, the functional

$$\tilde{Q}(\rho) = \inf\{(\psi, H_0 \psi) \mid \Psi \mapsto \rho\} \tag{1.8}$$

which was introduced by Levy[15] and analyzed by Lieb[11], has an obvious generalization to

$$Q(\rho) = \inf\{\mathrm{Tr}(\Gamma H_0) \mid \Gamma \mapsto \rho\} \tag{1.9}$$

This latter functional, which we use in Section 2, was introduced and studied by Lieb.[11]

This generalization suggests that one might hope that every ρ in $\mathscr{P}$ can be obtained from some ensemble density matrix Γ which is nonzero only on the span of the ground-state eigenspace of $H_0 + V$, i.e., $(H_0 + V)\Gamma = E_0 \Gamma$ and $\Gamma \mapsto \rho$. Unfortunately, even this seemingly modest expectation is false. As Englisch and Englisch[16] pointed out, even in the trivial case when $N = 1$, smooth densities may come from surprisingly singular potentials. The Englisch and Englisch counterexamples not only show that short-distance pathologies invalidate the above conjecture, but also suggest that the problem of completely characterizing range($\mathscr{R}$) is a difficult and subtle one indeed. Because of the importance of the Englisch and Englisch counterexamples, and also because we question the validity and interpretation of some of their examples, we comment in detail on their work in Section 5.

Finally, it should be noted (see, e.g. Lieb[11]) that the proof of the HK uniqueness theorem requires that if $\Psi \mapsto \rho$, then $\sum_\sigma |\Psi|^2 > 0$ a.e. This can be proved in the continuous case (via unique continuation theorems[12]) when the potential $v \mapsto \rho$ satisfies certain regularity conditions.

In Section 4, we consider uniqueness for quantum lattice systems. We establish the HK theorem for bosons at zero temperature. We also establish uniqueness for particles of any statistics in the finite-temperature case. The HK theorem for fermions at zero temperature remains an open problem.

2. EXISTENCE

We consider a system of $N < \infty$ particles on the d-dimensional lattice $\mathbb{Z}^d$. The particle interaction is described by a bounded, symmetric function

$$U: (\mathbb{Z}^d)^N \to \mathbb{R} \tag{2.1}$$

We note that this includes the case $U = \sum_{i<j} u(x_i - x_j)$, where u may be the Coulomb interaction for $d \geqslant 2$. The kinetic energy is given by a sum of single-particle finite difference Laplacians, which can be defined as

$$(-\Delta f)(x) = 2d f(x) - \sum_{y:|x-y|=1} f(y) \tag{2.2}$$

for any function $f: \mathbb{Z}^d \to \mathbb{C}$. Note that the lattice Laplacian is a *bounded* operator on the space of square-summable functions $l^2(\mathbb{Z}^d)$.

In the absence of an external potential, the Hamiltonian of the system is

$$H_0 = -\sum_{i=1}^{N} \Delta_i + U \tag{2.3}$$

Clearly, H_0 is a bounded operator on $l^2(\mathbb{Z}^d)^N)$.

An external potential is a function $v: \mathbb{Z}^d \to \mathbb{R}$. For a given v, the full Hamiltonian of the system is

$$H_v = H_0 + \sum_{i=1}^{N} v(x_i) \equiv H_0 + V \tag{2.4}$$

which is unbounded whenever v is.

The Hilbert space $\mathscr{H}$ on which H_0 acts is dictated by the statistics of the particles. For (spinless) bosons, $\mathscr{H} = \text{sym}[l^2((\mathbb{Z}^d)^N)]$, by which we denote the symmetric subspace of square-summable functions, i.e., symmetric N-particle wave functions. For spin-1/2 fermions, the system should be defined on $(\mathbb{Z}^d \otimes \{\alpha, \beta\})^N$. Thus we are concerned with antisymmetric square-summable functions $\varphi: (\mathbb{Z}^d \otimes \{\alpha, \beta\})^N \to \mathbb{C}$, so that $\mathscr{H} = \text{antisym}[l^2(\mathbb{Z}^d \otimes \{\alpha, \beta\})^N)]$. In the latter case, the Hamiltonians (2.4) which we study are spin independent. Henceforth we only consider wave functions in the appropriate symmetry subspace and omit explicit reference to symmetry constraints.

Note that, for any v, H_v has among its cores

$$\mathscr{B} = \{\varphi \in \mathscr{H} \mid \varphi = 0 \text{ except for finitely many points in } (\mathbb{Z}^d)^N\} \tag{2.5}$$

Since H_0 is bounded, the domain of H_v is simply

$$\mathscr{D}(V) = \left\{\varphi \in \mathscr{H} \;\middle|\; \sum_{x_1} \cdots \sum_{x_N} |(\varphi V)(x_1, ..., x_N)|^2 < \infty \right\} \tag{2.6}$$

H_v is clearly self-adjoint on $\mathscr{D}(V)$.

When v is bounded below, so is H_v, and the ground-state energy is given by

$$E_v = \inf\{(\varphi, H_v \varphi) \mid \varphi \in \mathscr{B}, \|\varphi\| = 1\} \tag{2.7}$$

There is a minimizing φ for (2.7) in $\mathscr{D}(V)$; it is said to be a ground state and satisfies $H_v \varphi = E_v \varphi$. For any given ground state φ, a density ρ_v in $l^1(\mathbb{Z}^d)$ may be constructed according to equation (1.3); for any set of (degenerate) ground states $\{\varphi_k\}$, a convex set of densities in $l^2(\mathbb{Z}^d)$ may be constructed via equations (1.4)–(1.6). We denote a generic element of this set by ρ_v.

We will consider densities in the set

$$\mathscr{P} = \left\{ \rho \colon \mathbb{Z}^d \to \mathbb{R}^+ \;\middle|\; \sum_x \rho = N, \quad \rho(x) > 0 \quad \text{and} \right.$$

$$\left. \begin{array}{lll} \rho(x) < N & \forall x \in \mathbb{Z}^d & \text{(bosons)} \\ \rho(x) < S & \forall x \in \mathbb{Z}^d & \text{(fermions)} \end{array} \right\} \qquad \begin{array}{r} (2.8\text{b}) \\ (2.8\text{f}) \end{array}$$

where S is the number of spin states. It is well known (see, e.g., Kuhn[17] or Coleman[18]) that (2.8) is sufficient to guarantee that for every ρ in $\mathscr{P}$ there exists a density matrix, Γ, of the proper symmetry such that $\Gamma \mapsto \rho$. If we were to replace $<$ by $\leqslant$ in the upper bounds in (2.8), these conditions would also be necessary for the existence of such a Γ. The physical interpretation of our restriction to strict inequality is that no potential which is finite at a particular site can attract particles so strongly to that site that it always contains the maximum number of particles; i.e., finite potentials do not allow Pauli saturation.

Given a $\rho \in \mathscr{P}$, we define the set of single-particle potentials

$$\mathscr{V}_\rho = \left\{ v \colon \mathbb{Z}^d \to \mathbb{R} \;\middle|\; \sum_x \rho\,|v| < \infty, E_v > -\infty \right\} \tag{2.9}$$

Note that $\mathscr{V}_\rho$ is nonempty since it contains all bounded functions.

The principal result of this section is the following.

Theorem 2.1. For any $\rho \in \mathscr{P}$, there exists a $\Gamma \mapsto \rho$ which is nonzero only on the ground-state eigenspace of H_v for some $v \in \mathscr{V}_\rho$.

We will give a variational proof of this theorem. To do this, for any fixed $\rho \in \mathscr{P}$, we consider the functional

$$\mathfrak{F}_\rho(v) = E_v - \sum_x \rho v \tag{2.10}$$

which is well defined for all v in $\mathscr{V}_\rho$. It is easy to verify that if $\mathfrak{F}_\rho$ has a maximizer v in $\mathscr{V}_\rho$, then $\rho = \rho_v$. Alternatively, $\mathfrak{F}_\rho$ is related to the functional $Q(\rho)$, defined in (1.9), by the following theorem, due to Lieb[11].

Theorem 2.2.

(a) $\sup\{\mathfrak{F}_\rho(v) \mid v \in \mathscr{V}_\rho\} = Q(\rho) \equiv \inf\{\mathrm{Tr}(\Gamma H_0) \mid \Gamma \mapsto \rho\}$ (2.11)

(b) There exists a Γ_0 which minimizes the right-hand side of (2.11), i.e., $Q(\rho) = \mathrm{Tr}(\Gamma_0 H_0)$, for some $\Gamma_0 \mapsto \rho$.

The utility of the functional $Q(\rho)$ is obvious from the above theorem. If it can be demonstrated that $\mathfrak{F}_\rho$ achieves a maximum v in $\mathscr{V}_\rho$, then the minimizer Γ_0 specified above must act on the ground-state eigenspace of H_v. The remainder of this section is devoted to the proof that $\mathfrak{F}_\rho$ achieves a maximum in $\mathscr{V}_\rho$.

By the Rayleigh–Ritz variational principle, for *any* $\Gamma \mapsto \rho$ we have

$$E_v \leqslant \mathrm{Tr}(\Gamma H_0) + \sum_x \rho v \tag{2.12}$$

which implies that $\mathfrak{F}_\rho(v)$ is bounded above uniformly in v by $\mathrm{Tr}(\Gamma H_0)$. Using the previous theorem of Lieb, we can state the following somewhat stronger result.

Proposition 2.3. $\mathfrak{F}_\rho$ is uniformly bounded above in $\mathscr{V}_\rho$, i.e.,

$$\sup\{\mathfrak{F}_\rho(v) \mid v \in \mathscr{V}_\rho\} = \mathrm{Tr}(\Gamma_0 H_0) \equiv Q(\rho) < \infty \tag{2.13}$$

Next, we recall that two potentials which differ only by a constant will have the same ground state, and note that

$$\mathfrak{F}_\rho(v + \text{const}) = \mathfrak{F}_\rho(v) \qquad \text{for all } v \text{ in } \mathscr{V}_\rho \tag{2.14}$$

Thus potentials which differ only a constant can be identified in HK theory. Henceforth, without loss of generality, we will consider only potentials for which the ground-state energy is zero, and use

$$\mathscr{V}_\rho^0 = \{v \in \mathscr{V}_\rho \mid E_v = 0\} \tag{2.15}$$

Theorem 2.4. Let $(v_k) \in \mathscr{V}_\rho^0$ be a maximizing sequence for $\mathfrak{F}_\rho$. Then there exists a v such that, for some subsequence,

$$v_k \to v \ \text{ pointwise} \tag{2.16}$$

This theorem depends on the following lemma, which will be proved separately for bosons and fermions.

Lemma 2.5. $\sum_k \rho\,|v_k|$ is bounded above uniformly in k.

Proof (for bosons). We will use the notation $v^+(x) = \max\{v(x), 0\}$ and $v^- = v^+ - v$ to denote the positive and negative parts of v, respectively.

Since (v_k) is a maximizing sequence

$$\lim_{k \to \infty} \sum_x \rho(v_k^+ - v_k^-) = -Q(\rho) \tag{2.17}$$

Let

$$D_k^+ = \sum_x \rho v_k^+, \qquad D_k^- = \sum_x \rho v_k^- \tag{2.18}$$

By (2.17), it is sufficient to verify that D_k^- is bounded above.

Let $B_k = \{x \mid v_k(x) < 0\}$. If $B_k = \varnothing$, then $D_k^- = 0$. Otherwise, let $n_k = N/\sum_{x \in B_k} \rho(x) \geqslant 1$. Define $\rho_k = n_k \rho \chi_{B_k}$, where $\chi_{B_k}(x) = 1$ if $x \in B_k$ and zero otherwise. Then there exists a (bosonic) density matrix $\Gamma_k \mapsto \rho_k$. By the condition $E_{v_k} = 0$, we have

$$0 \leqslant \mathrm{Tr}(\Gamma_k H_{v_k}) = \mathrm{Tr}(\Gamma_k H_0) - n_k D_k^- \leqslant \|H_0\| - D_k^- \tag{2.19}$$

which implies that D_k^- is uniformly bounded above. ■

Proof (for fermions). By assumption, the given ρ satisfies $\|\rho\|_\infty = S(1-\lambda)$ for some $0 < \lambda < 1$. Let B_k be defined as before. Let $b_k = \sum_{x \in B_k} \rho(x)$ and $a_k = \sum_{x \notin B_k} \rho(x)$. We distinguish two cases:

(i) If $a_k < \lambda N$, set

$$\rho_k = n_k \rho \chi_{B_k} \tag{2.20}$$

with n_k chosen so that $\sum_x \rho_k = N$. Then we have $n_k = N/b_k < 1/(1-\lambda)$, so that $\rho_k(x) < S$ for every x. Clearly $\rho_k(x) \geqslant 0$ for all x.

(ii) If $a_k \geqslant \lambda N$, set

$$\rho_k = n_k' \rho (1 - \chi_{B_k}) + (1+\lambda) \rho \chi_{B_k} \tag{2.21}$$

with n_k' chosen so that $\sum_x \rho_k = N$. It is easy to verify that $1 > n_k' \geqslant \lambda > 0$ so that $0 < \rho_k(x) < S$ for every x.

In both cases, ρ_k is nonnegative and satisfies (2.8f), so that we can find an N-particle (fermionic) density matrix Γ_k such that $\Gamma_k \mapsto \rho_k$. Therefore, a slight modification of the argument in (2.19) can be used to show that D_k^- is bounded above. In case (ii), one uses the fact that $\rho_k \leqslant \rho + \lambda \rho \chi_{B_k}$ to show $0 \leqslant \|H_0\| + \sum_x \rho v_k - \lambda D_k^-$, so that $\limsup_{k \to \infty} D_k^- \leqslant [\|H_0\| - Q(\rho)]/\lambda$. ■

Proof of Theorem 2.4. By Lemma 2.5, for every x

$$|v_k(x)| < \mathrm{const}/\rho(x) \tag{2.22}$$

For $x = 1$, choose a convergent subsequence and denote the limit by $v(1)$. Choose a further subsequence for $x = 2$, etc. This allows one to define a diagonal subsequence which converges pointwise (although not necessarily uniformly) to a limit function $v(x)$. ■

Theorem 2.6. The v defined by (2.16) is in $\mathscr{V}_\rho$. Moreover, $E_v \geqslant 0$.

Proof. By Fatou's lemma and Lemma 2.5,

$$\sum_x \rho v^+ \leqslant \lim_{k\to\infty} \sum_x \rho v_k^+ \tag{2.23}$$

which is bounded above, and similarly for v_-. Thus $\sum_x \rho\,|v| < \infty$.

For all $\varphi \in \mathscr{B}$, defined in (2.5), with $\|\varphi\| = 1$,

$$0 \leqslant \lim_{k\to\infty} (\varphi, H_{v_k}\varphi) = (\varphi, H_v\varphi) \tag{2.24}$$

which shows that H_v is nonnegative on a core and hence nonnegative on its domain. ■

Theorem 2.7. $H_{v_k} \to H_v$ in the strong resolvent sense.

Proof. The operators H_{v_k} and H_v are self-adjoint on their respective domains [defined by equation (2.6)]. For every φ in the common core $\mathscr{B}$

$$\|(H_{v_k} - H_v)\,\varphi\| \to 0 \tag{2.25}$$

which implies strong resolvent convergence (see, e.g., Theorem VIII.25 in Ref. 19). ■

Corollary. $e^{-H_{v_k}} \to e^{-H_v}$ in the strong operator sense.

Proof. We first note that whenever $A \geqslant 0$, e^{-A} can be obtained from a bounded continuous function on $\mathbb{R}$ using the standard operator calculus. Therefore since $E_{v_k}, E_v \geqslant 0$, this result follows immediately from well-known theorems (see, e.g., Theorem VIII.20 in Ref. 19). ■

Theorem 2.8. v maximizes $\mathfrak{F}_\rho$ in $\mathscr{V}_\rho$. Moreover, there is a $\Gamma_0 \longmapsto \rho$ which is nonzero only on a ground-state eigenspace of H_v.

Proof. Let Γ_0 be the minimizer given by Theorem 2.2(b). We first show that $\mathrm{Tr}(\Gamma_0 e^{-H_v}) = 1$. We have

$$\begin{aligned}
1 \geqslant \mathrm{Tr}(\Gamma_0 e^{-H_v}) &= \lim_{k\to\infty} \mathrm{Tr}(\Gamma_0 e^{-H_{v_k}}) \\
&\geqslant \exp[-\mathrm{Tr}(\Gamma_0 H_0)] \lim_{k\to\infty} \exp\left(-\sum \rho v_k\right) \\
&= e^{-Q(\rho)} e^{+Q(\rho)} \\
&= 1
\end{aligned} \tag{2.26}$$

The first inequality in (2.26) follows from the fact that $E_v \geqslant 0$. The second step is a consequence of the convergence established in the Corollary to Theorem 2.7. The third step follows from Jensen's inequality[10] applied to $\mathrm{Tr}(\Gamma_0 \cdot)$. The fourth step follows from the fact that for our maximizing sequence, $E_{v_k} = 0$ so that $\lim_{k\to\infty}(-\sum_x \rho v_k) = Q(\rho)$.

From $\mathrm{Tr}(\Gamma_0 e^{-H_v}) = 1$, it follows that $E_v = 0$ and Γ_0 is nonzero only on a ground-state eigenspace of H_v. Furthermore, since $\mathfrak{F}_\rho(v) = E_v - \sum_x \rho v$ and $E_v = \sum_x \rho v + \mathrm{Tr}(\Gamma_0 H_0) = 0$, we have $\mathfrak{F}_\rho(v) = Q(\rho)$, i.e., v maximizes $\mathfrak{F}_\rho$ in $\mathscr{V}_\rho$. ■

Remark. We note that the ground-state eigenfunctions implicitly defined by the previous theorem are actually in the domain of V and H_v, even though they were not constructed to be in $\mathscr{D}(V)$. Indeed *any* eigenfunction φ, with eigenvalue λ, of H_v is in $\mathscr{D}(V)$ since $|V\varphi|^2 = |(\lambda - H_0)\varphi|^2$ and H_0 is a bounded operator.

Remark. The arguments given above are also legitimate for a *finite* lattice $\Lambda \subset \mathbb{Z}^d$ provided that the Laplacian is supplemented with appropriate boundary conditions:

$$\Delta_\Lambda = \chi_\Lambda(x)\,\Delta \tag{2.27}$$

where χ_Λ is the characteristic function of the set Λ. (For fermions, it is immediately clear that Λ must contain more than N/S sites.)

3. EXISTENCE: FINITE-TEMPERATURE CASE

We again consider a system of $N < \infty$ particles on the lattice $\mathbb{Z}^d$ with Hamiltonian H_v given by (2.3)–(2.4). In this case, however, we are interested in the Gibbs state of a system at finite temperature $T = 1/\beta$.

For a given v, the partition function of the system is

$$Z_v(\beta) = \mathrm{Tr}(e^{-\beta H_v}) = \sum_j e^{-\beta E_j} \tag{3.1}$$

where the trace is taken over the appropriate symmetry subspace, and the E_j are the eigenvalues of H_v. Assuming that Z_v is finite, the Gibbs equilibrium state is given by the density operator

$$\Gamma_v = e^{-\beta H_v}/Z_v(\beta) \tag{3.2}$$

[10] The operator generalization of Jensen's inequality follows easily from the Klein or Peierls–Bogoliubov inequality.

This can be rewritten in the form (1.4) using the eigenfunctions of H_v in the usual way:

$$\Gamma_v(W, W') = \sum_j e^{-\beta E_j} \Psi_j(W)\, \bar{\Psi}_j(W')/Z_v(\beta) \tag{3.3}$$

The thermal density is given by

$$P_v(X) = \sum_{\sigma_1} \cdots \sum_{\sigma_N} \Gamma(W, W) \tag{3.4}$$

where $X = (x_1, ..., x_N)$. The single-particle density $\rho_v(x)$ is obtained by reducing Γ_v as in equations (1.3) and (1.6), or from P_v according to

$$\rho_v(x) = \sum_{x_2} \cdots \sum_{x_N} P_v(X) \tag{3.5}$$

We use the notation $\Gamma_v \mapsto P_v \mapsto \rho_v$.

For any density $\rho \in \mathscr{P}$, as defined in (2.8), let us consider the set of single-particle potentials

$$\mathscr{W}_\rho(\beta) = \left\{ v: \mathbb{Z}^d \to \mathbb{R} \;\middle|\; \sum_x \rho v < \infty, Z_v(\beta) < \infty \right\} \tag{3.6}$$

Since H_0 is bounded, it is easy to show that $Z_v(\beta) < \infty$ if and only if $\sum_x e^{-\beta v(x)} < \infty$. Therefore, the condition $Z_v(\beta) < \infty$ implies that $v(x)$ can take on negative values at only a finite number of lattice sites, so that $\sum_x \rho\, |v| < \infty$ if and only if $\sum_x \rho v < \infty$.

Here we address the question of whether or not there exists a $v \in \mathscr{W}_\rho(\beta)$ such that $\Gamma_v \mapsto \rho$. However, for thermal systems we will need to place an additional constraint on the densities ρ which we consider. The point is that, on physical grounds, we are interested in potentials v for which the Hamiltonian $H_v = H_0 + V$ satisfies

i. H_v has finite free energy, i.e., $\log Z_v(\beta) < \infty$; and
ii. the Gibbs state of H_v has finite energy, or equivalently, finite entropy.

The condition $Z_v(\beta) < \infty$ tales care of (i); however, it is not immediately clear that this condition does not also reduce $\mathscr{W}_\rho(\beta)$ to the empty set, since any v in $\mathscr{W}_\rho(\beta)$ must be unbounded. We will see that the requirement that $\mathscr{W}_\rho(\beta)$ be nonempty also takes care of (ii). The following theorem shows that $\mathscr{W}_\rho(\beta)$ is nonempty if and only if the entropy-like quantity $-\sum_x \rho(x) \log \rho(x)$ is finite. As we explain in the Appendix, this is *precisely* the condition needed in order that the entropy of the N-particle Gibbs state be finite.

Theorem 3.1. For any $\rho \in \mathscr{P}$, the following two statements are equivalent:

(a) $T(\rho) \equiv -\sum_x \rho(x) \log \rho(x) < \infty$

(b) $\mathscr{W}_\rho(\beta) \neq \varnothing$.

Proof. First recall that

$$Z_v(\beta) < \infty \Leftrightarrow \sum_x e^{-\beta v(x)} < \infty \tag{3.7}$$

Using this, it is clear that the potential $v(x) = -\log \rho(x)/\beta$ satisfies $Z_v(\beta) < \infty$. Furthermore, if $T(\rho) < \infty$, then $\sum_x \rho v < \infty$ so that $v \in \mathscr{W}_\rho(\beta)$, i.e., (a) implies (b).

Next, recall that the convexity of $f(t) = t \log t$ implies that $a \log a - a \log b \geqslant a - b$. For v in $W_\rho(\beta)$ we let $b = e^{-\beta v(x)}$ and $a = \rho(x)$. Summing over x proves that (b) implies (a). ■

The previous theorem suggests that we consider the set of densities given by

$$\mathscr{P}^T = \left\{ \rho \in \mathscr{P} \;\middle|\; -\sum_x \rho \log \rho < \infty \right\} \tag{3.8}$$

The principal result of this section is the following.

Theorem 3.2. For any $\rho \in \mathscr{P}^T$, there exists a $v \in \mathscr{W}_\rho(\beta)$ such that $\Gamma_v \mapsto \rho$.

As in the previous section, the proof of this theorem is variational. For any $\rho \in \mathscr{P}^T$, we define the functional

$$\mathfrak{G}_\rho(v) = \exp\left(-\beta \sum_x \rho v\right) \Big/ Z_v(\beta) \tag{3.9}$$

Note that $\mathfrak{G}_\rho$ is well-defined for all $v \in \mathscr{W}_\rho(\beta)$.

Proposition 3.3. $\mathfrak{G}_\rho$ is uniformly bounded above in $\mathscr{W}_\rho(\beta)$.

Proof. Let $v \in \mathscr{W}_\rho(\beta)$. Construct $\Gamma \mapsto \rho$. Then, by Jensen's inequality applied to $\mathrm{Tr}(\Gamma\, \cdot)$, we have

$$Z_v \geqslant \mathrm{Tr}(\Gamma e^{-\beta H_v}) \geqslant e^{-\beta\, \mathrm{Tr}(\Gamma H_0)} e^{-\beta \Sigma \rho v} \geqslant e^{-\beta \|H_0\|} e^{-\beta \Sigma \rho v} \tag{3.10}$$

Thus $\mathfrak{G}_\rho(v) \leqslant e^{\beta \|H_0\|}$. ■

Theorem 3.3. $\mathfrak{G}_\rho$ achieves a maximum in $\mathscr{W}_\rho(\beta)$.

Proof. Let (v_k) be a maximizing sequence for $\mathfrak{G}_\rho$ in $\mathscr{W}_\rho(\beta)$. Without loss of generality, we may normalize the v_k so that $\mathrm{Tr}(e^{-\beta H_{v_k}}) = 1$ for every

k. We remark that with this normalization, the ground-state energy is nonnegative for all k.

Following exactly the proofs of Theorem 2.4, Lemma 2.5, Theorem 2.6, and Theorem 2.7, we conclude that, for some subsequence, there exists a v such that

i. $v_k \to v$ pointwise;
ii. $v \in \mathscr{W}_\rho(\beta)$; and
iii. $e^{-\beta H_{v_k}} \to e^{-\beta H_v}$ in the strong operator sense.

In order to show that the v defined by (i) maximizes $\mathfrak{G}_\rho$, we first note that either (3.10) or Lemma 2.5 can be used to show that $(\rho v_k)(x)$ is bounded below uniformly in k and x. Thus, by Fatou's lemma

$$\lim_{k\to\infty} \sum_x \rho v_k \geqslant \sum_x \rho v \tag{3.11}$$

Furthermore, by (iii) and the operator form of Fatou's lemma (see, e.g., Ref. 20),

$$\lim_{k\to\infty} \operatorname{Tr}(e^{-\beta H_{v_k}}) \geqslant \operatorname{Tr}(e^{-\beta H_v}) \tag{3.12}$$

Combining (3.11) and (3.12), we have

$$\mathfrak{G}_\rho(v) \geqslant \lim_{k\to\infty} \mathfrak{G}_\rho(v_k) = \sup\{\mathfrak{G}_\rho(v) \mid v \in \mathscr{W}_\rho(\beta)\} \quad \blacksquare \tag{3.13}$$

The principal result (Theorem 3.2) now follows from a standard variational argument established below.

Theorem 3.4. If v maximizes $\mathfrak{G}_\rho$ in $\mathscr{W}_\rho(\beta)$, then $\rho(x) = \rho_v(x)$.

Proof. Let $\eta: \mathbb{Z}^d \to \mathbb{R}$ be a function which vanishes on all but finitely many points of $\mathbb{Z}^d$. Then, for $\varepsilon \in \mathbb{R}^+$, $v + \varepsilon\eta \in \mathscr{W}_\rho(\beta)$, so that

$$\mathfrak{G}_\rho(v + \varepsilon\eta) \leqslant \mathfrak{G}_\rho(v) \tag{3.14}$$

Then, by the Golden–Thompson inequality (see, e.g., Ref. 20)

$$\begin{aligned} \operatorname{Tr}(e^{-\beta H_{v+\varepsilon\eta}}) &\leqslant \operatorname{Tr}\left(e^{-\beta H_v} \prod^N e^{-\beta\varepsilon\eta}\right) \\ &= Z_v \left[1 - \varepsilon\beta \sum_x \rho_v \eta\right] + o(\varepsilon) \end{aligned} \tag{3.15}$$

while

$$e^{-\beta\Sigma\rho(v+\varepsilon\eta)} = e^{-\beta\Sigma\rho v}\left[1 - \varepsilon\beta \sum_x \rho\eta\right] + o(\varepsilon) \tag{3.16}$$

Thus

$$\mathfrak{G}_\rho(v+\varepsilon\eta) \geqslant \mathfrak{G}_\rho(v)\left[1-\varepsilon\beta\sum_x (\rho-\rho_v)\,\eta\right]+o(\varepsilon) \tag{3.17}$$

which, by proper choice of η, violates (3.14) if ρ and ρ_v differ at any site. ■

Remark. As noted in Section 2, these results hold for finite lattices provided that the Laplacian is supplemented with suitable boundary conditions.

4. UNIQUENESS

In this section, we address the question of whether or not the v giving rise to a particular density ρ is unique (up to a constant). The standard HK proof of uniqueness for continuous systems[1] relies on assumptions concerning the zeros of ground-state eigenfunctions (see Lieb[11]). In particular, the proof reduces to the statement that two potentials of the form $V=\sum_i v(x_i)$ cannot be identical on the set of points, $X=(x_1,\ldots,x_N)$, for which the corresponding wave function Ψ (or density matrix) satisfies

$$\sum_\sigma |\Psi(X)|^2 > 0 \qquad \text{a.e.} \tag{4.1}$$

That this is true for a large class of potentials (presumably $v\in L^{3/2}_{\text{loc}}$, see Ref. 21) follows from unique continuation theorems (see, e.g., Ref. 12). However, in density functional theory, the class of potentials is normally *not* specified *a priori*. Indeed, it is easy to construct densities from potentials which do not satisfy the hypotheses of the unique continuation theorem. Thus, a complete proof of the HK theorem, that is a proof which allows the inclusion of such general potentials, has not been given for continuous systems.

If the ground state is known to be nonzero, the standard HK uniqueness arguments can be extended to zero-temperature quantum lattice systems. Thus we conclude that $V=\sum_i v$ is unique whenever the corresponding ground-state wave functions satisfy (4.1). For bosons, strict positivity of the ground-state wave function can be shown by Perron–Fröbenius arguments (see, e.g., Ref. 12). Thus we have the following theorem.

Theorem 4.1. For zero-temperature bosonic lattice systems, the potential $v(x)$ giving rise to the density $\rho_v(x)$ is unique (up to a constant).

Furthermore, strict positivity of $\rho(x)$ implies that strict inequality in (2.8b) is necessary so that the conditions in Theorem 2.1 are necessary, as well as sufficient. Therefore, we conclude that in the case of bosons there is a map[11]

$$\mathscr{R}: l^+(\mathbb{Z}^d) \to \mathscr{P} \tag{4.2}$$

from positive potentials on $\mathbb{Z}^d$ to strictly positive, properly normalized densities, which is one-to-one and onto.

In the case of fermions, the situation is more complex and, as yet, unresolved. The HK uniqueness theorem is obviously false for N fermions with S spin states on a lattice with precisely N/S sites. In this trivial case, only one antisymmetric function exists so that *all* potentials have the same ground state and, therefore, the same density. In general, (4.1) will not hold because antisymmetry forces the wave function to vanish at many points, any one of which must be thought of as "open" or having nonzero measure. However, the relevant question is not whether (4.1) is satisfied at *every* point $X = (x_1,..., x_N)$, but whether there are *enough* points on which some ground-state wave function does not vanish to conclude that $v(x)$ is unique. Although this is quite plausible, we do not know of any proof.

Regarding the related question of whether or not the strict inequality, $0 < \rho(x) < S$, is necessary in the case of fermions, we know of no direct proof. However, in addition to the physical argument given earlier, the existence of a ρ in range($\mathscr{R}$) for which $\rho(x_0) = 0$ or $\rho(x_0) = S$ at *some* lattice site x_0 would contradict the widely believed conjecture that range($\mathscr{R}$) is open. For finite lattices, arguments analogous to Kohn's proof[9] of openness would appear to eliminate the possibility of Pauli saturation.

At finite temperature, uniqueness is true for quantum lattice systems with any statistics. This does not follow from HK arguments, but by showing that $\mathfrak{G}_\rho$ has a unique maximizer.

Theorem 4.2. Assume v_1, $v_2 \in \mathscr{W}_\rho(\beta)$ both maximize $\mathfrak{G}_\rho$. Then $v_1(x) = v_2(x) + \text{const}$.

Proof. Let $v = 1/2(v_1 + v_2)$. Clearly, $\sum_x \rho v < \infty$. By the Golden–Thompson (see, e.g., Ref. 20) and Cauchy–Schwarz inequalities

$$\mathrm{Tr}(e^{-\beta H_v}) \leqslant [\mathrm{Tr}(e^{-\beta H_{v_1}})\, \mathrm{Tr}(e^{-\beta H_{v_2}})]^{1/2} \tag{4.3}$$

and thus $v \in \mathscr{W}_\rho(\beta)$. Furthermore (4.3) implies

$$\mathfrak{G}_\rho(v) \geqslant [\mathfrak{G}_\rho(v_1)(\mathfrak{G}_\rho(v_2)]^{1/2} \tag{4.4}$$

[11] $l^+(\mathbb{Z}^d) = \{$all positive, real-valued functions on $\mathbb{Z}^d$, modulo constants$\}$.

Evidently v also maximizes $\mathfrak{G}_\rho$. This implies that Cauchy–Schwarz must be saturated, which means that

$$e^{-H_{v_1}} = (\text{const})\, e^{-H_{v_2}} \tag{4.5}$$

Since $v_1, v_2 \in \mathscr{W}_\rho(\beta)$, this implies

$$H_{v_1} - H_{v_2} = V_1 - V_2 = \text{const} \quad \blacksquare \tag{4.6}$$

Corollary. For finite-temperature lattice systems, the potential $v(x)$ giving rise to the density $\rho_v(x)$ is unique (up to a constant).

Proof. By the Hölder inequality applied to $\mathrm{Tr}(e^{-\beta H_v})$, it is clear that $\mathfrak{G}_\rho$ is log concave in v (see, e.g., Ref. 20). Thus, by the above theorem, it can have at most one critical point. $\blacksquare$

Finally, we note that the necessity of strict inequality in (2.8) in Theorem 3.2 can easily be seen using straightforward orthogonality arguments.

5. THE ENGLISCH AND ENGLISCH COUNTEREXAMPLES

Englisch and Englisch[16] (EE) considered the validity of the following statement.

Inverse Conjecture: For every density ρ in $\mathscr{P}$, there is a real-valued potential v such that a normalized density matrix Γ, which is nonzero only on the ground-state eigenspace of $H_0 + V$ [i.e., $(H_0 + V)\Gamma = E_v \Gamma$], satisfies $\Gamma \longmapsto \rho$.

They give a negative answer by means of several counterexamples which we analyze below.

EE construct their examples for the simple case when $N = 1$ (or, equivalently, for N bosons when the interaction $U = 0$). In this case, the ground state is nondegenerate, and the density is $\rho = |\Psi|^2$, where Ψ is the ground-state eigenfunction. We can assume without loss of generality that $\Psi = \sqrt{\rho}$ and that the ground-state energy is zero. Then the eigenvalue equation is $(-\Delta + v)\sqrt{\rho} = 0$. Since $\rho > 0$, v, if it exists, must be given by $v = \Delta\sqrt{\rho}/\sqrt{\rho}$.

For such v, we observe that

$$\begin{aligned}\int |\varphi|^2 (\Delta\sqrt{\rho})/\sqrt{\rho} &= -\int \nabla(|\varphi|^2/\sqrt{\rho}) \cdot \nabla\sqrt{\rho} \\ &= \int \rho \left| \nabla \left(\frac{\varphi}{\sqrt{\rho}} \right) \right|^2 - \int |\nabla\varphi|^2 \end{aligned} \tag{5.1}$$

so that, at least formally,

$$(\varphi, (-\Delta + v)\,\varphi) = \int \rho \left| \nabla \left(\frac{\varphi}{\sqrt{\rho}} \right) \right|^2 \geqslant 0 \tag{5.2}$$

which is consistent with the assumption that the ground-state energy is zero. While it is certainly conceivable that $\Delta \sqrt{\rho}$ may be singular enough to invalidate the integration by parts in (5.1), we do expect to be able to find a dense set of φ which avoid the singularities so that the above argument is still valid. We also expect such φ to define a core for $-\Delta + v$, so that can conclude that $-\Delta + v$ is a positive operator. Therefore, we regard the claim of EE that a v of the form $\Delta \sqrt{\rho}/\sqrt{\rho}$ can define a Hamiltonian which is unbounded below with caution and skepticism.

For this reason, we believe that EE's example 5 in Ref. 16, which is based on the long-distance behavior of ρ, is incorrect. In fact, the above argument can be rigorously applied to the functions φ_i defined in their equation (38) to show that $(\varphi_i, (-\Delta + v)\,\varphi_i) \geqslant 0$, contrary to their claim. Indeed, since we could expect any such long-distance problems to also manifest themselves on the lattice, our results suggest that *long-distance difficulties do not generally occur in HK theory*. Therefore we turn our attention to the more interesting short-distance examples.

EE first consider a one-dimensional example which is explicitly defined only near $x = 0$. Their example 4 in Ref. 16 is given by

$$\rho = (a + b\,|x|^{\alpha + 1/2})^2$$

where $|x| < 1$, $a > b > 0$, and $1/2 > \alpha > 0$. If one insists that the potential be a real-valued function, the only possible candidate is

$$v(x) = b(\alpha^2 - 1/4)\,|x|^{\alpha - 3/2}/\sqrt{\rho} \sim -b'\,|x|^{\alpha - 3/2}$$

where $b' > 0$. For this v, $-\Delta + v$ is unbounded below as EE claim, in apparent contradiction to our remarks above. However, v is not formally given by $\Delta \sqrt{\rho}/\sqrt{\rho}$, because

$$\Delta \sqrt{\rho} = b(\alpha + 1/2)\,|x|^{\alpha - 1/2}\,\delta(x) + b(\alpha^2 - 1/4)\,|x|^{\alpha - 3/2}$$

Thus it appears that ρ is associated with the ground state of a Hamiltonian whose potential is not a real-valued function, but a distribution.[12] Thus EE have constructed a ρ in $\mathscr{P}$ that does not satisfy the conjecture. This ρ is not the ground state of any Hamiltonian $-\Delta + v$, having a real-valued potential,

[12] Differentiation of $|x|$ can be avoided by considering, e.g., $\rho = (a + bx^{3/5})^2$ but the resulting potential goes as $-b'x^{-7/5}$, which is odd around the singular point. This prevents $-\Delta + v$ from being unbounded below.

although it may be the ground state of a Hamiltonian with a distributional potential.

This example suggests that we ought to look more closely at the relationship between the domain and range of the function $\mathscr{R}(v)$ which maps $v \to \rho$. Although we have devoted considerable attention to the problem of characterizing range($\mathscr{R}$), we have been surprisingly cavalier about its domain. The problem with $\mathscr{R}$ is that it need not map smooth $\leftrightarrow$ smooth. It may map very singular potentials into very smooth densities. Indeed, one of the principal difficulties with characterizing range($\mathscr{R}$) in the continuous case is that reasonable choices for domain($\mathscr{R}$) do not go to equally reasonable subsets of $\mathscr{P}$. This problem did not occur for the lattice because it is possible to choose, as we implicitly did, domain($\mathscr{R}$) $= l^+(\mathbb{Z}^d) =$ {all positive, real-valued functions on $\mathbb{R}^d$}.

At this point it may seem tempting to try to circumvent the difficulties of EE's example 4 by extending the domain of $\mathscr{R}$ to include generalized potentials. However, we caution the reader that much of HK theory, particularly the proof of the basic uniqueness theorem, may break down for generalized potentials.

Although the first counterexample is sufficient to settle the conjecture, some additional insight into the problem can be gained by studying a generalization of one of EE's other examples. In this case,

$$\rho(x) = [a + bx^p \sin(x^{-s})]^2$$

near $x = 0$, where $a > |b| > 0$ and $s \geqslant 1$. This example may be either one dimensional or three dimensional, where in the latter case we assume that ρ is spherically symmetric and identify x with $|\mathbf{r}|$. For $d = 1$, EE considered an example of this form with $s = 1$ and x^p replaced by $|x|^p$. Here we avoid differentiating $|x|$ by assuming p is a (positive) fraction with odd denominator (e.g., $p = 3/5$) and s is a (positive) integer. For both $d = 1$ and $d = 3$, the most singular part of v goes as $b'x^{p-2s-2} \sin(x^{-s})$. If we now require

$$s \geqslant 1 \qquad s + 1 < p < 2s + 1 \qquad (d = 1)$$

$$s > 2 \qquad s + 1 < p < 2s - 1 \qquad (d = 3)$$

the lower bound implies that $\nabla \sqrt{\rho}$ is continuous at $x = 0$, which is more than sufficient to ensure $\sqrt{\rho} \in H_1$. However, the upper bound implies that $\int |\Psi|^2 |v| = \int \rho |v| = \infty$ in both cases. Thus $\sqrt{\rho}$ is not in the form domain of v. However, $\int \rho v$ can be defined as a limit, which suggests that $\sqrt{\rho}$ may be the ground state of a self-adjoint extension of $-\Delta + v$. In fact, it follows easily from a theorem of Combescure and Ginibre[26,27] that such H_v are essentially self-adjoint, so that one does not get counterexamples of this type.

Now consider only $d=1$ and let $s+1/2<p<s+1$ (e.g., $s=1$, $p=5/3$). Then $\sqrt{\rho}\in H^1$, but both $\nabla\sqrt{\rho}$ and $\Delta\sqrt{\rho}$ are undefined at the origin; $\int \rho\,|v|=+\infty$ and it is not at all obvious how one should define $\int \rho v$. This suggests that $\sqrt{\rho}$ may not be in the form domain or the Friedrich's extension of $-\Delta+v$. Thus, the question of whether or not this example contradicts the conjecture involves some subtle and unpleasant domain questions.

These examples obviously do not extend to our lattice systems because they involve short-distance pathologies which cannot occur for a discrete system. Furthermore, the domain questions associated with the sum $-\Delta+v$ cannot occur on the lattice even if v is very singular as $|x|\to\infty$, because the finite difference Laplacian is *bounded*. Domain problems arise when one takes the sum of *two* unbounded operators. If one attempts to extend our proofs to continuous systems, one encounters domain problems of this type head-on.

APPENDIX: FINITE ENTROPY CONDITIONS

We wish to show that the condition $T(\rho)<\infty$, used in Section 3, is equivalent to the requirement that we restrict ourselves to N-particle Gibbs states with finite entropy. Because the sum over spins in (3.4) does not play an essential role, for simplicity we will limit our discussion to spinless bosons.

Recall that the entropy of the density matrix, Γ is defined as

$$\begin{aligned} S(\Gamma) &= -\mathrm{Tr}\,\Gamma\log\Gamma \\ &= -\sum_k \lambda_k \log\lambda_k \end{aligned} \tag{A.1}$$

where the λ_k are the eigenvalues of Γ. For lattice systems, one can also define the quantity

$$T(P) = -\sum_X P(X)\log P(X) \tag{A.2}$$

which measures the amount of disorder in the distribution of particles over lattice sites. In general, Γ is not diagonal, so that $T(P)\neq S(\Gamma)$. However, concavity of the entropy implies that

$$S(\Gamma)\leqslant T(P) \tag{A.3}$$

(see, e.g., Wehrl,[22] Section I.B.5).

We now wish to relate $S(\Gamma)$ and $T(P)$ to the corresponding single-particle quantities, $S(\gamma)$ and $T(\rho)$. Although T is not a quantum mechanical entropy, it has all the properties of an entropy. Indeed, (3.4) implies that

$T(P)$ acts like the entropy of a classical discrete system. (For an excellent summary of entropy inequalities which compares classical discrete, classical continuous, and quantum entropies, see Lieb,[23] especially properties C and D. Note that the densities, $\hat{\rho}$, in Ref. 23 are normalized to 1, and that $T(\rho) = T(N\hat{\rho}) = NT(\hat{\rho}) - N \log N$, etc.). In particular, if $P \mapsto \rho$

$$T(P) \geqslant \frac{1}{N} T(\rho) + \log N \tag{A.4}$$

and

$$T(P) \leqslant T(\rho) + N \log N \tag{A.5}$$

The monotonicity (A.4) follows from Jensen's inequality; (A.5) follows from repeated use of subadditivity. These inequalities clearly imply that $T(P)$ is finite if and only if $T(\rho)$ is finite for any $\Gamma \mapsto \rho$.

By combining (A.3) and (A.5), we immediately see that whenever $T(\rho)$ is finite, any N-particle system which reduces to ρ has finite entropy since

$$S(\Gamma) \leqslant T(P) \leqslant T(\rho) + N \log N \tag{A.6}$$

whenever $\Gamma \mapsto P \mapsto \rho$. We could also have reached the same conclusion via

$$\begin{aligned} S(\Gamma) &\leqslant S(\gamma) + N \log N \\ &\leqslant T(\rho) + N \log N \end{aligned} \tag{A.7}$$

whenever $\Gamma \mapsto \gamma \mapsto \rho$. Note that (A.7) also shows $S(\gamma) < \infty$ implies $S(\Gamma) < \infty$ whenever $\Gamma \mapsto \rho$.

We now wish to consider the converse question: Does finite entropy for an N-particle system imply that the corresponding $S(\gamma)$ and/or $T(\rho)$ are finite? At first glance the answer appears to be no, since it is easy to find examples of pure states, Γ, for which $S(\gamma) = T(\rho) = +\infty$ $(\Gamma \to \gamma \to \rho)$ although $S(\Gamma)$ is necessarily zero. If, however, we restrict ourselves to Gibbs states, Γ_v, corresponding to Hamiltonians $H = H_0 + \sum_i v(x_i)$ of the type under consideration in this paper, the answer is positive. In that case

$$\begin{aligned} S(\Gamma_v) &= \beta \langle H_v \rangle + \log Z_v(\beta) \\ &= \beta \operatorname{Tr}(H_0 \Gamma_v) + \beta \sum_x \rho v + \log Z_v(\beta) \end{aligned} \tag{A.8}$$

Thus, if ρ is V-representable, then $S(\Gamma_v) < \infty$ implies that $v \in \mathscr{W}_\rho(\beta)$, which by Theorem 3.1 implies $T(\rho) < \infty$.

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