Coarse-grained spin density-functional theory: infinite-volume limit via the hyperfinite

Paul E. Lammert
Dept. of Physics, 104B Davey Lab
Pennsylvania State University
University Park, PA 16802-6300

(Dated: 1 May 2014)

Coarse-grained spin density functional theory (SDFT) is a version of SDFT which works with number/spin densities specified to a limited resolution — averages over cells of a regular spatial partition — and external potentials constant on the cells. This coarse-grained setting facilitates a rigorous investigation of the mathematical foundations which goes well beyond what is currently possible in the conventional formulation. Problems of existence, uniqueness and regularity of representing potentials in the coarse-grained SDFT setting are here studied using techniques of (Robinsonian) nonstandard analysis. Every density which is nowhere spin-saturated is V-representable, and the set of representing potentials is the functional derivative, in an appropriate generalized sense, of the Lieb internal energy functional. Quasi-continuity and closure properties of the set-valued representing potentials map are also established. The extent of possible non-uniqueness is similar to that found in non-rigorous studies of the conventional theory, namely non-uniqueness can occur for states of collinear magnetization which are eigenstates of $S_z$.

PACS numbers: 31.15.Ew, 02.30.Sa, 71.15.Mb

1. INTRODUCTION

Modern electronic density functional theory\cite{1,2} (DFT) is a very successful basis for the computation of ground state properties used by chemists, physicists and materials scientists. However, it is not just practical computational algorithms, but also a distinctive way of looking at quantum many-body systems with its own set of fascinating basic questions.

While the computational side of DFT is highly developed, the mathematical foundations are relatively impoverished. The fundamental questions revolve around the concept of V-representability. For a system of $N$ electrons, with their mutual Coulomb repulsion, a single-particle density $\rho(x)$ is said to be pure-state V-representable if some external single-particle potential $v(x)$ has a ground state wavefunction with single-particle density $\rho$. It is mixed-state V-representable (simply “V-representable” here) if there is a mixed ground state (density matrix) with density $\rho$. Natural questions are those of existence, uniqueness and regularity of the representing potentials as a function of density. The realization that some densities are not pure-state V-representable, but are mixed-state V-representable was responsible for the rise to prominence of the latter concept\cite{5,6} around 1980. About the same time, some densities which are not even mixed-state V-representable were suggested\cite{7}. Although V-representable densities are dense in an appropriate topology, so are non-V-representable densities and there is as yet no nontrivial positive characterization of V-representability. Concerning uniqueness, the original paper of Hohenberg and Kohn\cite{1} already contained a strong uniqueness result (modulo a trivial constant shift of the potential). Subsequently, when the theory was generalized to spin density functional theory (SDFT) in order to study magnetic phenomena, it was realized\cite{8} that there was some breakdown of uniqueness in that context. There has recently been clarification\cite{9,10} of the extent of that nonuniqueness. Questions of regularity — how much will the representing potential of a density resemble those of nearby densities — has been almost entirely neglected. And not just by a lack of results; even the question seems largely unacknowledged. These foundational issues are also relevant to the computational side of DFT. Computability is threatened not only by lack of existence, but also by lack of regularity.

Chayes, Chayes and Ruskai\cite{11} studied DFT for a lattice version of quantum mechanics and showed that, although serious mathematical difficulties or even pathologies may arise from the presence of arbitrarily short distance scales, the infinite-volume limit is a tractable problem. In particular, it was shown that every density is a ground-state density of an essentially unique potential. On a lattice, short distance scales are completely eliminated; this is a fundamentally different quantum mechanics than the orthodox continuum version. Another way to keep short-distance-scale degrees of freedom from causing problems without altering the underlying continuum quantum mechanics was introduced as coarse-grained DFT\cite{12}. The idea is that we only allow ourselves to specify densities with some limited spatial resolution. On scales finer than the resolution, the density is automatically relaxed by an energetic criterion. This approach seems much in the spirit of DFT. Conventional density functional theory asks for the lowest-intrinsic-energy (kinetic plus Coulomb) state consistent with a fully and exactly specified density. But it is entirely natural, and perhaps more computationally relevant, to consider incomplete specifications. Unique V-representability holds also in this formulation and fur-
ther regularity results were recently demonstrated. Although the infinite-volume limit was handled, it was not found to be trivial, and for each property had to be approached anew. Since practical computations work with limited representational resources, usually in a form that amounts to limited spatial resolution, the coarse-grained formulation might be considered a more suitable grounding than the conventional fine-grained one. On the other hand, the coarse-graining scale can be taken as small as one wishes (10^{-30} m, say), so the approach is not inherently imprecise. Still, the infinite-resolution limit in which the coarse-graining scale goes to zero is of interest to understand the scale-dependences and to make contact with things formulated in a conventional infinite-resolution form such as an exact Coulomb potential. For that limit the coarse-grained formulation seems to have an advantage over the lattice, since a finer scale on the lattice requires a new lattice, not just some extra resolution. Some progress in that vein has been made for ordinary (non-spin) DFT. This paper has no new contribution concerning that problem, but instead returns to the single-scale setting and the infinite-volume limit for spin-density functional theory.

In previous work on the coarse-grained approach, it was observed that for a system confined to a finite box the situation really is simple. This paper aims to explore the situation brought by the infinitesimal methods allows not just ordinary DFT, but also spin density functional theory to be handled. Everything is done from scratch; there is no dependence on the earlier results. Thus, this paper also aims to promote the use of infinitesimal methods, which are not nearly as well-known as they deserve. It is hoped that nonstandard analysis will in the future allow the continuum limit also to be dealt with.

The next section reviews some basic ideas of SDFT and Section 2 is a very brief introduction to nonstandard analysis (NSA). Readers with appropriate background can skip these sections. Section 3 gets down to work, proving some fundamental lower semicontinuity and near-standardness results using infinitesimal tools. The basic ideas and notations for the coarse-grained formulation are given in the short Section 4.

The main results of the paper are found in Secs. 5, 7 and 8. The coarse-grained versions of the Lieb internal energy functional \( F[\rho] \) and the set-valued function \( \text{Potl}(\rho) \) which gives the representing potentials are the main objects of interest. Section 6 proves that \( F \) is continuous, that \( \text{Potl}(\rho) \) is non-empty if \( \rho \) is everywhere non-zero and nowhere spin-saturated, that \( \text{Potl}(\rho) \) is the functional derivative of \( F \) in a sense appropriate to a general convex functional, that the map \( \rho \to \{ \rho \cdot v : v \in \text{Potl}(\rho) \} \) restricted to nowhere spin-saturated densities is an \( L^1 \) upper semicontinuous set-valued function and that the graph of \( \text{Potl} \) is closed. The reason we have to work with \( \text{Potl} \) as a set-valued function is the well-known non-uniqueness in the SDFT context. Sections 7 and 8 deal with this problem. There are no nonstandard arguments in these sections, so they could probably be read on their own. The extent of non-uniqueness in the coarse-grained theory is shown to coincide with earlier non-rigorous conclusions for the continuum theory. Namely, number/spin potentials may be non-unique only if the spin-density is saturated somewhere, or in case of collinear magnetization in an eigenstate of \( S_z \). The appropriate conditions are formulated in terms of densities rather than wavefunctions. Some concluding remarks are found in Section 9. Sections 7 and 8 have a very different flavor from that of Sections 4, 5, and 6, but they are all important parts of a well-rounded picture.

The reader who is curious about the nonstandard arguments might consider reading quickly through Section 4 and then skipping to Sections 7 and 8. The reader who just wants to see the results may wish to start with the summary at the beginning of Section 9. Working backwards as needed.

2. SOME BASIC IDEAS OF SDFT

In this section, we review some basic ideas of non-relativistic Density Functional Theory. It can safely be skipped by anyone with an acquaintance with that formalism, after taking note of our notation for spin densities. The discussion is kept at a heuristic level.

We are concerned with a system of \( N \) identical particles interacting with each other and subject to an external single-particle potential which functions as a control parameter. The wavefunction of a pure state for this system is a function \( \psi(z_1, z_2, \ldots, z_N) \) of \( N \) positions \( x_\alpha \) and \( N \) spin components \( s_\alpha \) with respect to some quantization axis. These are combined in the abbreviated notation \( z_\alpha = (x_\alpha, s_\alpha) \). In the usual concrete situations, the particles are electrons interacting via Coulomb repulsion. These are spin-1/2 fermions, so that there are no antisymmetric functions under interchange of \( z_\alpha \) and \( z_\beta \) for \( \alpha \neq \beta \). The value of the particles’ spin, and even whether they are fermions or bosons plays no crucial role. The discussion in this paper is tailored to the spin-1/2 fermion case, but appropriate modifications can be made for others. With the inner product

\[
\langle \psi|\phi \rangle = \int \psi^*(z)\phi(z) \, dz_1 \cdots dz_N,
\]

where \( \int dz \) denotes integration over position and summation over spin, the antisymmetric wavefunctions comprise an \( L^2 \) Hilbert space which will be denoted \( \mathcal{H} \).
As alluded to in the introduction, a general Density Functional Theory working only with pure states does not get very far. For reasons of convexity\footnote{This is an extremely important property and a nice way to rephrase it is in terms of the epigraph of $F$, \[ \text{epi} F := \{ \langle \rho', y \rangle : y \geq F[\rho'] \}, \] which is the region on or above the graph of $F$ in $X \times \mathbb{R}$. Thus, epi $F$ is a convex set. It is also closed in the $L^1$ topology\footnote{see Cor. 1.2}; this property corresponds to lower semicontinuity of $F$. A representing potential $v$ for $\rho$ is a four-component function defined by the property \[ F[\rho] + \langle v, \rho \rangle \leq F[\rho'] + \langle v, \rho' \rangle \quad \forall \rho' \in X. \] The notation $\langle v, \rho \rangle$ means \[ \langle v, \rho \rangle := \int v \cdot \rho \, dx = \int (v_0 \rho_0 + \vec{v} \cdot \vec{\rho}) \, dx. \]}

it is advantageous to allow mixed states, also called density matrices; this is also a physically reasonable extension. Mathematically, a mixed state is represented by a positive trace class operator in $\mathcal{B}$, having an eigenfunction expansion of the form

$$\gamma = \sum_{i=1}^{\infty} c_i |\psi_i\rangle \langle \psi_i|, \quad (2)$$

in Dirac notation, where $|\psi_i\rangle$ is an orthonormal set.

The (single-particle) number/spin density corresponding to pure state $\psi$ is

$$\rho_{\alpha\beta}(x) = N \int dz \cdots dz_N \psi(x, z_2, \ldots, z_N)^* \psi(x, z_2, \ldots, z_N). \quad (3)$$

This is a $2 \times 2$ matrix-valued function of position. With $\sigma_0$ the $2 \times 2$ unit matrix and $\sigma_1, \sigma_2, \sigma_3$ the Pauli matrices, the number/spin density can be written as

$$\rho = \rho_0 \sigma_0 + \rho_1 \sigma_1 + \rho_2 \sigma_2 + \rho_3 \sigma_3 = \sum_{\alpha<\beta} \frac{1}{2} \text{Tr} (\sigma_\alpha \rho) \sigma_\beta. \quad (4)$$

It is therefore convenient to express the number/spin density as the four-vector

$$\rho := (\rho_0, \vec{\rho}) = (\rho_0, \rho_1, \rho_2, \rho_3), \quad (5)$$

and refer to it as the 4-density, the first component being number density and last three proportional to the spin density. An alternative notation $(n, 2\vec{n}) = (\rho_0, \vec{\rho})$ will also be used, mostly in Sections 7 and 8. The factor of 2 means that $\vec{n}$ actually integrates to the spin in units of $\hbar$.

The 4-density satisfies $|\vec{n}| \leq \rho_0/2$ everywhere. Notation like $|\psi \mapsto \rho^\prime|$ is customarily used to indicate that $\psi$ gives the 4-density $\rho$, but this is sometimes awkward, so we give the map a name. The 4-density corresponding to $\psi$ is denoted $\text{Dens} \gamma$. This state-to-density map extends additively to mixed states; that is,

$$\text{Dens} \gamma = \sum_i c_i \text{Dens} \psi_i.$$ 

A physically normalized pure state satisfies $\|\psi\| = 1$, so that $\int \rho_0 \, dx = N$. Constantly making sure of the normalization is a distracting and unecessary nuisance. Thus, we do not generally assume or insist that states and densities be physically normalized, unless otherwise noted.

It is traditional to work with the ingredients of the Hamiltonian as Hilbert space operators, but quadratic forms are mathematically convenient and arguably more physically meaningful. Define the kinetic energy quadratic form by

$$\mathcal{E}^K(\psi, \phi) := \frac{1}{2} \int \nabla \psi(\vec{z})^* \cdot \nabla \phi(\vec{z}) \, d\vec{z}. \quad (6)$$

the Coulomb interaction energy quadratic form by

$$\mathcal{E}^C(\psi, \phi) := \sum_{\alpha<\beta} \int \frac{1}{|x_\alpha - x_\beta|} \phi(\vec{z}) \, d\vec{z}, \quad (7)$$

and the total intrinsic energy by

$$\mathcal{E}(\psi, \phi) := \mathcal{E}^K(\psi, \phi) + \mathcal{E}^C(\psi, \phi). \quad (8)$$

For the moment, we ignore domain questions. The abbreviation $\mathcal{E}(\psi, \phi) = \mathcal{E}(\psi)$ is used for diagonal elements, and similarly for $\mathcal{E}^K$ and $\mathcal{E}^C$.

The Lieb internal energy functional\footnote{see Cor. 1.2} for SDFT is defined by

$$F[\rho] := \inf \{ \mathcal{E}(\gamma) : \gamma \in \mathcal{S}, \text{Dens} \gamma = \rho \}. \quad (9)$$

This is the minimum intrinsic energy consistent with density $\rho$. The Lieb functional is simple and natural in retrospect, but took a long time to emerge. It solved the original “$V$-representability problem”, by extending the Hohenberg-Kohn internal energy functional to densities regardless of $V$-representability (indeed, without any mention of potentials). To discuss the continuity of $F$, this most central object of DFT, requires a topology. One which suggests itself is the $L^1$ norm topology which is implicit in the very concept of density. In other words, we view the 4-densities as a subset of $X := L^1(\mathbb{R}^3; \mathbb{C}^4)$ with the norm

$$\|f\| = \int (|f_0(x)| + |\vec{f}(x)|) \, dx. \quad (10)$$

Then, $F$ is extended to all of $X$ with value $+\infty$ off the range of the Dens map; this is just a convenience with no physical significance. There are highly oscillatory densities in the range of Dens for which $F = +\infty$, as well.

Because the Lieb functional is defined in terms of mixed states rather than pure states, it is easy to see that $F$ is convex:

$$F[\lambda \rho + (1 - \lambda) \rho'] \leq \lambda F[\rho] + (1 - \lambda) F[\rho'], \quad (11)$$

for $0 \leq \lambda \leq 1$. This is an extremely important property and a nice way to rephrase it is in terms of the epigraph of $F$.

$$\text{epi} F := \{ (\rho, y) : y \geq F[\rho'] \},$$

which is the region on or above the graph of $F$ in $X \times \mathbb{R}$. Thus, epi $F$ is a convex set. It is also closed in the $L^1$ topology\footnote{see Cor. 1.2}; this property corresponds to lower semicontinuity of $F$.

A representing potential $v$ for $\rho$ is a four-component function defined by the property

$$F[\rho] + \langle v, \rho \rangle \leq F[\rho'] + \langle v, \rho' \rangle \quad \forall \rho' \in X. \quad (12)$$
Physically, $\bar{\rho}$ may be thought of as a magnetic field, though its divergence is unconstrained.

It appears at first sight that some abstract results of convex analysis\textsuperscript{11,22} can be applied to the situation. For example, the Hahn-Banach theorem asserts the existence of a closed hyperplane separating $(\rho, F[\rho])$ from the interior of epi $F$. Such a hyperplane would be the geometrical counterpart of a representing potential for $\rho$ in $X^*$, the dual space of $X$. Similarly, there is a theorem (Prop. I.5.3 of\textsuperscript{11}) which says that when there is a unique such hyperplane at $(\rho, F[\rho])$, then it is the Gâteaux derivative of $F$ at $\rho$, if $F$ is continuous at $\rho$. Unfortunately, these theorems get no traction whatever because $F$ is not continuous. In fact, the effective domain of $F$, $\text{dom} F = \{ \rho \in X : F[\rho] < +\infty \}$ has empty interior. This is easy to see\textsuperscript{21,22}. Any open ball around any point in $X$ contains elements of $X$ which are negative somewhere, hence not even in dom $F$. In addition, adding short-wavelength wiggles to a density can drive its kinetic energy arbitrarily high, or even to infinity, with arbitrarily small change in $\rho$. Lieb\textsuperscript{11} took $L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$ for $X$ instead of $L^1(\mathbb{R}^3)$. $L^3$ does not contain the full range of Dens, but it does contain the densities of finite internal energy, so is acceptable. This choice of $X$, however, does not solve the problems just mentioned. Furthermore, there are reasonable potentials which are not even linear functionals. For instance, a harmonic potential $|x|^2$ takes value $+\infty$ on some densities. Eq. (12) makes perfect sense for such a case.

The only general result on V-representability in the conventional framework is the fact\textsuperscript{11,22} that the set of densities which are representable by a potential in $X^*$ is dense in dom $F$ in $X$-norm. This is a very weak result, and does not appear to be useful.

Given a pair $\rho, \mathbf{v}$ satisfying Eq. (12), $\mathbf{v}$ can be regarded as some sort of “derivative” of $F$ at $\rho$. But what sort? In particular, we would like to know whether $(−\mathbf{v}, \delta \rho)$ coincides with the directional derivatives

$$F'(\rho, \delta \rho) := \lim_{\epsilon \to 0} \frac{1}{\epsilon} (F[\rho + \epsilon \delta \rho] - F[\rho]).$$

(14)

There is no general guarantee of this, as suggested above in reference to Gâteaux differentiability.

The questions just raised — which densities are V-representable (not to mention, just what qualifies as a potential)? to what extent do representing potentials coincide with directional derivatives of $F$? — are basic elements of an inquiry into the characteristics, potentially pathological, of the internal energy functional $F$. At least insofar as computational algorithms applied to practical problems are iterative, these questions are relevant, since the behavior of $F$ in a full neighborhood of a sought density is so. The rest of this paper aims at, and obtains, satisfactory answers to these questions in a coarse-grained framework, which is slightly different and less demanding than the conventional fine-grained one discussed in this section. Formally, everything is very similar, as the changes amount to a reinterpretation of density and potential. With a little nonstandard analysis, the answers for the coarse-grained theory are obtained easily. The next section therefore gives a whirlwind tour of the basics of nonstandard analysis.

3. SOME BASIC IDEAS OF NSA

In the 1960’s Abraham Robinson\textsuperscript{23} revived the old idea of infinitesimals using methods from model theory (a branch of mathematical logic), and thereby creating the field of Nonstandard Analysis or infinitesimal analysis. Although they are a characteristic feature, however, infinitesimals are far from the only “ideal” objects Nonstandard Analysis offers for dealing with mathematical problems. In this section, I try to prepare the reader with just enough of the jargon and basic ideas that the flavor of arguments in the rest of the paper may be appreciated. This flavor — once one gets used to it — is highly intuitive. For further background, I highly recommend the notes of Lindstrom\textsuperscript{24}. For a highly compressed (twelve-page) summary, see Section 1 of\textsuperscript{22}. There are also several good books,\textsuperscript{25} as well as some resources available on the web.

In (model theoretic) nonstandard analysis, there is a nonstandard counterpart of every conventional mathematical object. A natural place to start is with the traditional reals, $\mathbb{R}$. Its counterpart is $\ast \mathbb{R}$, the ordered field of hyperreals, which is an extension of $\mathbb{R}$: in addition to the familiar real numbers, $\ast \mathbb{R}$ contains infinitesimals and their reciprocals, the illimited hyperreals. $\epsilon \in \ast \mathbb{R}$ is infinitesimal if $|\epsilon| < \delta$ for every $\delta > 0$ in $\mathbb{R}$, whereas $x$ is illimited (called “infinite” by many) if $|x| > n$ for every natural number $n$. The notation “$n \approx +\infty” (n \approx -\infty)” means that $n$ is positive (negative) illimited, and $x \ll \infty$ means that $x$ is limited.

Two hyperreals $x$ and $y$ are infinitely close, $x \approx y$, if their difference is an infinitesimal. Thus, “$x$ is infinitesimal” and “$x \approx 0$” are synonymous. $x \lesssim y$ means that $x$ does not exceed $y$ by more than an infinitesimal.

In fact, every object (formally viewed as a set) of conventional mathematics has a nonstandard enrichment. The enrichment of the naturals is $\ast \mathbb{N}$, the hypernaturals. $\ast \mathbb{N}$ contains $\mathbb{N}$, as well as illimited hypernaturals.

Not only objects, but (first order) mathematical statements have $\ast$-transforms. Consider a sequence $(x_n)_{n \in \mathbb{N}}$ of real numbers. It has a $\ast$-transform which is a map from $\ast \mathbb{N}$ to $\ast \mathbb{R}$, and which we continue to denote by $x_n$. The statement “$\lim_{n \to \infty} x_n = a”$, is equivalent to “given $k \in \mathbb{N}$, there is $m_k$ such that $\forall n \in \mathbb{N}$, $n > m_k \Rightarrow |x_n - a| < 1/k^k$. $\mathbb{N}$, $a$ and $m_k$ are parameters in this statement. Since $\ast a = a$ and $\ast m_k = m_k$, the $\ast$-transform of the statement is $\forall n \in \ast \mathbb{N}$, $n > m_k \Rightarrow |x_n - a| < 1/k^k$. To obtain the $\ast$-transform, just “put stars on everything”.

The point of the operation is that the Transfer Principle asserts that statement in the standard universe is true if and only if its $\ast$-transform is true in the nonstandard universe. In the case at hand, an illimited $n$ will satisfy
all the statements as \( k \) runs through \( \mathbb{N} \), so \( x_n \approx a \) for illimited \( n \). And conversely, if \( x_n \approx a \) for illimited \( n \), \( a \) is the limit of the original sequence.

In a similar way, one finds the nonstandard characterization of continuity for a function \( f : \mathbb{R} \to \mathbb{R} \). Namely, for \( x \in \mathbb{R} \) and \( y \in \mathbb{R} \) with \( y \approx x \), \( f(y) \approx f(x) \). As just happened with \( *f(y) \), stars will sometimes be dropped when no ambiguity is possible. If \( x \) is standard and \( y \approx x \), then \( x \) is the standard part of \( y \), and we write \( x = \hbar y \) or \( x = \hbar st \). For a standard point \( x \), the collection of all points infinitesimally close to it is called its monad. Continuity of \( f \) at \( x \) is equivalent to \( f \) maps the monad of \( x \) into the monad of \( f(x) \). These concepts of monad and standard part generalize to arbitrary topological spaces.

For another example, consider the least number principle:

\[ \forall B \in \mathcal{P}(\mathbb{N}), \exists x \in B : y \in B \Rightarrow x \leq y. \]

This has \( * \)-transform

\[ \forall B \in *\mathcal{P}(\mathbb{N}), \exists x \in B : y \in B \Rightarrow x \leq y. \]

The one free parameter, \( \mathcal{P}(\mathbb{N}) \), the power set of the naturals, has been replace by \( *\mathcal{P}(\mathbb{N}) \). This is \( * \) not the power set of \( *\mathbb{N} \). Instead, it is the set of internal subsets of \( *\mathbb{N} \). A set is standard if it is the \( * \)-transform of a conventional set, for example \( *\mathbb{N} \). A set is internal if it is an element of a standard set. Standard sets are also internal. Not all subsets of \( *\mathbb{N} \) are internal. For example, \( *\mathbb{N} \setminus \mathbb{N} \) is not. Indeed, if \( n \) is illimited, so is \( n - 1 \). Thus, since the set of illimited hypernaturals does not obey the least number principle, it must not be internal. It is external. Similar reasoning leads to the conclusion that the set of infinitesimals in \( *\mathbb{R} \), or the monad of any point, is an external set.

The internal/external dichotomy is subtle, but crucially important. If \( A \) is an internal subset of \( *\mathbb{N} \) containing all illimited \( n \), then there must be some limited \( m \) such that \( n \geq m \Rightarrow n \in A \). This consequence of the least number principle is called underflow (or underspill). Similarly, an internal subset of \( *\mathbb{N} \) containing all sufficiently large limited numbers contains also some illimited numbers (overflow or overspill), and an internal subset of \( *\mathbb{R} \) containing all non-negative infinitesimals contains all \( x < \epsilon \) for some \( \epsilon > 0 \) in \( \mathbb{R} \).

How can we recognize internal sets, apart from the definition? The Internal Definition Principle gives an answer. If \( A \) is an internal set and \( \phi(x; A, B_1, \ldots, B_n) \) is a formula with internal parameters \( A, B_1, \ldots, B_n \), then the subset of \( A \) consisting of the elements satisfying \( \phi \), \( \{ x \in A : \phi(x; A, B_1, \ldots, B_n) \} \) is also internal. Suppose an internal sequence \( (x_n)_{n \in \mathbb{N}} \) is given with the property that \( x_n \approx 0 \) for all limited \( n \). Then, the set \( \{ m \in *\mathbb{N} : |x_m| < 1/m \} \) is internal. The parameters in it are \( *\mathbb{N} \) and \( (x_n) \), both of which are internal. Thus, this set is internal by the Internal Definition Principle, and therefore contains all \( m \) up to some \( N \) in \( *\mathbb{N} \setminus \mathbb{N} \), implying that \( x_m \approx 0 \) for all \( m \leq N \). ("Robinson’s Lemma")

Another important principle is Saturation. For an infinite cardinal \( \kappa \), a \( \kappa \)-saturated nonstandard model has the property that, if \( \{ A_j \}_{j \in J} \) is a collection of internal sets with an index set of cardinality less than \( \kappa \) and the finite intersection property, then \( \cap_{j \in J} A_j \neq \emptyset \). Usually \( N_1 \)-saturation is adequate for applications. We assume that much, at least.

The sequence space \( \ell_1 \) and its nonstandard enrichment is a prototype of some of the spaces which will be used later. By definition, \( \ell_1 \) is the Banach space of sequences \( x : \mathbb{N} \to \mathbb{C} \) with finite norm \( \|x\| = \sum_{j=1}^{\infty} |x_j| < \infty \). Then, \( *\ell_1 \) consists of sequences \( *\mathbb{N} \to *\mathbb{C} \) with norm \( \|y\| = \sum_{j \in *\mathbb{N}} |y_j| \) mapping \( *\ell_1 \) into \( *\mathbb{R} \). If \( x \) is standard, (in \( \ell_1 \)) then \( y \) is in the monad of \( x \) \( (y \approx x) \) if \( \|y - x\| = \sum_{j \in *\mathbb{N}} |y_j - x_j| \approx 0 \). Here, the \( * \) has been dropped on the nonstandard extensions of both the standard element \( x \) and the norm. We seek a more explicit condition ensuring \( y \approx x \).

\( y \) is said to be nearstandard if it is in the monad of some standard vector in \( \ell_1 \), which must therefore be its standard part \( \hbar y \). I claim that \( y \) is nearstandard precisely when \( \|y\| \) is limited and \( y \) “has infinitesimal tail”: \( \sum_{i \geq n} |y_i| \approx 0 \) for all illimited \( n \). And, in that case the standard part of \( y \) is given by

\[ (**y)_i = \hbar (y_i), \]  

for limited \( i \). (15)

The first condition is obvious. The second follows from the fact that a standard \( x \in \ell_1 \) has infinitesimal tail: given \( k \in \mathbb{N} \), there is \( N_k \) such that \( n \geq N_k \Rightarrow \sum_{i \geq n} |x_i| < 1/k \). By Transfer, \( n \approx +\infty \) satisfies all of these statements as \( k \) varies, and therefore \( \sum_{i \geq n} |x_i| \approx 0 \). (The \( * \) on \( \hbar x \) has been dropped again.) So, \( y \approx x \) implies \( y \) also has infinitesimal tail. All that remains to verify, then, is that (15) gives the standard part. Define \( x \in \ell_1 \) by \( x_i = \hbar (y_i) \) for limited \( i \). Then, given any natural \( k \), the set \( A_k = \{ n : \sum_{i < n} |y_i - x_i| < 1/k \} \) contains all \( n \in \mathbb{N} \). It is also internal, since it has two standard parameters \( (k) \) and \( (x) \) and one internal but nonstandard parameter \( (y) \). Thus, there is an illimited \( N \) in \( A_k \). But then, \( \sum_{i < N} |y_i - x_i| = \sum_{i < N} |y_i - x_i| + \sum_{i \geq N} |y_i - x_i| \approx 1/k \) because \( N \in A_k \) and both \( y \) and \( x \) have infinitesimal tail. This being true for every \( k \), \( \|y - x\| \approx 0 \) and \( x \approx y \), the standard part of \( y \).

The nonstandard characterizations of open, closed and compact subsets of a topological space are simple and useful. \( st^{-1}A \) denotes the union of the monads of all points of \( A \). \( A \) is open if \( st^{-1}A \subset *A \), it is compact if \( *A \subset st^{-1}A \), and it is closed if \( st^{-1}A \) contains all nearstandard points in \( *A \).

4. LOWER SEMICONTINUITY AND NEARSTANDARD MIXED STATES

This Section establishes lower semicontinuity of the energy forms introduced in Sec. 2 both for pure states and mixed states. Some of the consequences, particularly
Corollaries 4.1 and 4.2 will be important later. The results are somewhat technical, but are a nice illustration of nonstandard methods.

We begin with a nonstandard approach to lower semicontinuity of \(E\) on \(S\), which is a case of the equivalence of closedness and lower semicontinuity of positive quadratic forms\[^{35}\]. Returning to the quadratic forms \([0,1]\)regard them as initially defined on the space of (antisymmetric) \(C^\infty\) valued infinitely differentiable functions of rapid decrease at infinity (the components correspond to spin indices). That is, \((1 + |x|^2)^m \partial^a f/\partial x^a\) is bounded for all \(m\) and multi-indices \(\alpha\). Denote this “seed space” by \(S\); other choices work, but this one has especially nice properties with respect to Fourier transformation.

It is very important that the form \(E^\zeta\) is bounded relative to \(E^K\) with relative bound less than \(1^{36,38}\), that is, for some \(0 < a < 1\), a sufficiently large \(b\) can be found such that

\[
E^\zeta(\psi) \leq aE^K(\psi) + b\|\psi\|^2. \tag{16}
\]

This means that the non-degenerate inner product

\[
\langle x|y\rangle_E = E(x,y) + \langle x|y\rangle
\]

is equivalent to \(\langle x|y\rangle_K\), defined similarly but with \(E\) replaced by \(E^K\). That means that there is some \(c > 0\) satisfying \(c^{-1}\langle x|y\rangle_K \leq \langle x|y\rangle_E \leq c\langle x|y\rangle_K\). One nonstandard way to construct the completion of \(S\) with respect to \(\langle x|y\rangle\) or \(\langle x|y\rangle_K\) is as a weak nonstandard hull. This abstract construction actually applies to completion of any linear space \(S\) with respect to a non-degenerate inner product. Let \(W\) be the collection of seminorms \(x \mapsto \|x\|_E\) for \(\phi \in S\), initially defined as real-valued on \(S\), but immediately extended to hyperreal seminorms on \(*S\). Now define the set of \(W\)-infinitesimal elements \(\text{inf}_W*S\) of \(*S\) to be those satisfying \(\|x|\phi\| \approx 0\) for every \(\phi \in S\), and the \(W\)-finite elements \(\text{fin}_W*S\) those satisfying \(\|x|\phi\| \ll \infty\) for every \(\phi \in S\). The completion of \(S\) is obtained as the quotient \(\hat{S} = \text{fin}_W*S/\text{inf}_W*S\), and the norm is \(\|x\| = \sup\{\|x|\phi\|: \phi \in S, \|\phi\| = 1\}\). It is clear that \(S\) can be viewed as a subset of \(\hat{S}\) by identifying elements with their equivalence classes. To see that \(\hat{S}\) is complete, consider a Cauchy sequence \((x_n)\) in \(\hat{S}\), lifting to a sequence \((x_n)\) in \(*S\). By overspill and countable enumeration, the sequence can be extended up to \(N \in *N, N\) still respecting the Cauchy condition \(m > k_n \Rightarrow \|x_m - x_k\| < 1/n\) for each \(n\) in \(N\). Thus, \(x_N\) is the sought limit of the sequence in \(\hat{S}\).

If \(\hat{S}\) is taken to be the \(L^2\) completion of \(S\), then this construction makes it clear that \(S\) is \(\hat{S}\), the completion of \(S\) with respect to \(E^K\) norm can be identified with a subspace of \(\hat{S}\). For, since \(\langle x|\phi\rangle_K = (x|H_{00}\phi)\), where \(H_{00}\) is the kinetic energy Hamiltonian (well-defined as a map \(S \rightarrow S\)), \(\langle \cdot | \cdot \rangle\) monads are no larger than \(\langle \cdot | \cdot \rangle_K\) monads. On the other hand, they are also obviously no smaller due to the relative weakness of the \(\parallel \cdot \parallel\) norm compared to the \(\parallel \cdot \parallel_K\) norm.

On \(\hat{S}\), the ordinary \(L^2\) and \(E^K\) norms can be found according to \(\|x\| = f(x), \|x\|_K = f_K(x)\), where \(f(x) : = \|\phi(x)\| : \phi \in S, \|\phi\| = 1\), and \(f_K(x) : = \|\phi(x)|_K : \phi \in S, \|\phi\|_K = 1\). These take values in \([0,\infty]\). Since each seminorm \(x \mapsto \|\phi(x)|_K = \|H_{00}\phi(x)|\) is weakly continuous, the supremum is lower semicontinuous. Another way to this conclusion is to look at the function \(f_K\) on \(\hat{S}\): \(f_K(x) = \sup\{\|\phi(x)|_K : \phi \in S, \|\phi\|_K = 1\}\). Now, if \(x\) is standard, that is to say, in \(S\), then \(f(x) = f(x)\). For \(x \approx x\), \(\|\phi(x)|_K \approx \|\phi(y)|_K\) for every \(\phi \in S\), yet the supremum defining \(\|y_0|_K\) includes also \(\phi \in \hat{S}\) so that \(\|y_0|_K \gtrsim \|x\|_K\) which is exactly the nonstandard characterization of lower semicontinuity.

**Lemma 4.1.** \(E_1\) is lower semicontinuous on \(\hat{S}\)

**Proof.** The proof is contained in the preceding two paragraphs. Also, see Reference\[^{32}\].

Turning to mixed states, \(\Gamma \in *\hat{S}\) is nearstandard if it is nearstandard with respect to trace-norm (the only topology we consider on \(\hat{S}\)). It will be useful to characterize this more concretely in terms of nearstandardness in \(*\hat{S}\). Whenever possible and profitable we try to reduce properties of mixed states to corresponding, but more intuitively graspable properties of pure states. Now, note that for \(\gamma = \sum_{i \in N} c_i |\psi_i\rangle\langle \psi_i|\) in \(\hat{S}\), given \(c \geq 0\) in \(\mathbb{R}\), there is a finite-range mixed state within \(\epsilon\) of \(\gamma\) in trace norm. Indeed, some truncation \(\sum_{i=1}^m c_i |\psi_i\rangle\langle \psi_i|\) will serve the purpose. Otherwise put, the finite-range mixed states are dense in \(\hat{S}\). Thus, a mixed state \(\gamma = \sum_{i \in N} c_i |\psi_i\rangle\langle \psi_i|\) in \(*\hat{S}\) is nearstandard if and only if it can be approximated to any given standard accuracy by some partial sum \(\sum_{i \in J} |\psi_i\rangle\langle \psi_i|\) with \(|J| < \infty\). With the terms of the sum ordered by decreasing eigenvalue, this is equivalent to: \(\psi_i\) is nearstandard whenever \(c_i \neq 0\), and \(\sum_{i=1}^\infty c_i = \text{Tr}\gamma\). Also, note that trace-norm topology is stronger than uniform topology, which in turn is stronger than strong-operator topology, so that \(\gamma \approx \gamma\) only if every eigenvector of \(\gamma\) is infinitesimally close to being an eigencector of \(\gamma\) with the same eigenvalue: if \((\gamma - a|\psi\rangle\langle \psi|) = 0\), then \((\gamma - a|\psi\rangle\langle \psi|) = 0\).

The way is now prepared for the analog of Lemma 4.1 for mixed states.

**Lemma 4.2.** \(E_1\) is lower semicontinuous on \(\hat{S}\)

**Proof.** Take \(\gamma \in \hat{S}\), with nonstandard enrichment \(\gamma = \sum_{i \in N} c_i |\psi_i\rangle\langle \psi_i|\), and suppose \(\gamma = (\sum_{i \in N} c_i |\psi_i\rangle\langle \psi_i)|\) satisfies \(\gamma \approx \gamma\). We need to show that \(E_1(\gamma_1) \gtrsim E_1(\gamma)\). As just discussed, every eigenvector \(\psi_i\) of \(\gamma\) is infinitely close to an eigenvector \(\psi_i\) of \(\gamma\) with infinitely close eigenvalue, and vice versa. But, since the eigenvectors of \(\gamma\) are standard, Lemma 4.1 implies that

\[
E_1(\psi_i) \gtrsim E_1(\psi_i) = E_1(\psi_i).
\]

(We assume that the terms are arranged in decreasing order of eigenvectors and in case of equal eigenvalues,
appropriate choices of basis must be made.) Thus,
\[ \sum_{i=1}^{m} c_{i}^{*}E_{1}(\psi_{i}) \gtrsim \sum_{i=1}^{m} c_{i}E_{1}(\psi_{i}), \]
for any \( m \in \mathbb{N} \). From this, we immediately conclude that
\( E_{1}(\gamma') \gtrsim E_{1}(\gamma) \).

The map \( \text{Dens} \) from \( \mathcal{H} \) to \( L^{1} \) is continuous, therefore if \( \psi \in \mathcal{H} \) is nearstandard, \( \text{Dens} \psi \) is also \( L^{1} \)-nearstandard. Going the other way, a weaker condition on \( \text{Dens} \psi \), together with energy-boundedness of \( \psi \) suffices to guarantee nearstandardness of \( \Psi \) as we shall see.

If for any \( \epsilon > 0 \), there is some \( R \) such that \( \int_{x \geq R} \rho \, dx < \epsilon \), we will say that \( \rho \) is “nearstandardly concentrated”. Note that, by underspill this is equivalent to \( \int_{x \geq R} \ast \rho \, dx \approx 0 \) for all illimited \( R \).

**Lemma 4.3.** If \( \Psi \in \mathcal{H} \) has nearstandardly concentrated density and \( E_{1}(\Psi) \) is limited, then \( \Psi \) is nearstandard.

**Proof.** Note that, since \( \mathcal{H} \) is a complete metric space, it suffices to show that \( \Psi \) can be approximated to any standard accuracy by a vector in \( \mathcal{H} \). Also, by relative form boundedness of \( \mathcal{E} \) with respect to \( \mathcal{E}^{K} \), together with positivity of \( \mathcal{E}^{C} \), there is some constant \( c \) such that \( c^{-1}E_{1} < E_{1}^{K} < cE_{1} \), so that \( \mathcal{E} \) and \( \mathcal{E}^{K} \) are interchangeable for our purposes here.

The first step is to show that \( \Psi \) can be approximated by a *\( \mathcal{H} \) vector with bounded support and finite energy (a “smooth truncation”). Then we will be able to assume that \( \Psi \) itself is a vector with no loss of generality. So, let \( \chi(x) \) be a smooth cutoff function which is nonincreasing with \( \|x\| \), equal to one in \( B_{1} \) and supported in \( B_{2} \), where \( B_{R} \) is the ball \( \|x\| \leq R \). For \( R > 0 \), define the \( N \)-particle cutoff function by
\[ \hat{\chi}_{R} = \prod_{\alpha=1}^{N} \chi(x_{\alpha}/R), \]
and cutoff wavefunction by
\[ \Phi_{R} = \hat{\chi}_{R}\Psi. \]

Thus, \( \Phi_{R} \) has zero probability for any particle to be outside the \( 2R \)-ball. By the assumption of nearstandardly concentrated density, \( \|\Phi_{R} - \Psi\| \) can be made smaller than any standard tolerance by taking \( R \) large enough. Further, since \( \nabla\Phi_{R} = \hat{\nabla}_{R}\nabla\Psi + (\hat{\nabla}_{R}\Psi) \) and \( \hat{\chi}_{R} \) is smooth, \( \mathcal{E}_{1}^{K}(\Phi_{R}) \) is limited. Thus, we may assume that \( \Psi \) has bounded support, contained in the closed box \( \mathcal{B}_{L} = \{ |x|, |y|, |z| \leq L \} \), and now consider that case.

Using the particle-in-a-box wavefunctions for \( \mathcal{B}_{L} \), we can construct an explicit orthonormal basis for \( \mathcal{H}_{L} \), the closed subspace of \( \mathcal{H} \) consisting of vectors with density supported in \( \mathcal{B}_{L} \). For any \( E \), there are a finite number of basis vectors with \( \mathcal{E}_{L}^{K} < E \). Thus, given any \( E \) and \( \epsilon \), there is a finite orthonormal set \( \psi_{1}, \ldots, \psi_{n} \) such that whenever \( \phi \in \mathcal{H}_{L} \) satisfies \( E_{1}(\phi) < E \), then the component of \( \phi \) orthogonal to \( \text{span}(\psi_{1}, \ldots, \psi_{n}) \) has norm less than \( \epsilon \). By Transfer, this continues to hold for \( \phi \in \ast \mathcal{H}_{L} \).

But, the projection of \( \phi \) onto \( \text{span}(\varphi_{1}, \ldots, \varphi_{n}) \) is clearly nearstandard. Since \( E \) and \( \epsilon \) are free, this means that \( \Psi \) can be approximated to any standard tolerance by a nearstandard vector, and therefore is itself nearstandard.

Here is the central result of this Section.

**Proposition 4.1.** If, for \( \Gamma \in \ast \mathcal{G} \), \( \text{Dens} \Gamma \) is nearstandardly concentrated and \( E_{1}(\Gamma) \) is limited, then \( \Gamma \) is nearstandard.

**Proof.** Let \( \Gamma \) have eigenfunction expansion
\[ \Gamma = \sum_{i \in \mathbb{N}} c_{i}\langle \psi_{i} \rangle \langle \psi_{i} \rangle. \]

Since \( \text{Dens} \) and \( E_{1} \) are additive and positive maps, whenever \( c_{i} \) is not infinitesimal, \( \psi_{i} \) is nearstandardly concentrated and of limited energy, hence nearstandard by Lemma 4.3. Thus, with
\[ \Gamma' := \sum_{i=1}^{\infty} \ast c_{i}\langle \psi_{i} \rangle \langle \psi_{i} \rangle, \]

it follows that \( \ast \Gamma = \Gamma' \) unless the sum of infinitesimal weights \( c_{i} \) is noninfinitesimal, that is \( \text{Tr} \Gamma' < \text{Tr} \Gamma - \epsilon \), for some \( \epsilon > 0 \) in \( \mathbb{R} \). In that case, defining \( J_{n} := \{ i : c_{i} < 1/n \} \), the internal set \( K := \{ n \in \mathbb{N} : \sum_{J_{n}} c_{i} > \epsilon \} \) contains all of \( \mathbb{N} \), hence some illimited \( \omega \), and \( |J_{\omega}| > \epsilon \omega \).

Now define the mixed state
\[ \tilde{\Gamma} := \sum_{i \in J_{\omega}} c_{i}\langle \psi_{i} \rangle \langle \psi_{i} \rangle < \Gamma. \]

Since \( \mathcal{H} \) is separable, fewer than \( \epsilon \omega/2 \) of the (orthogonal) eigenvectors \( \psi_{i} \) of \( \tilde{\Gamma} \) can be nearstandard, and they carry a combined weight not exceeding \( (\epsilon \omega/2)(1/\omega) = \epsilon/2 \). The remaining eigenvectors are not nearstandard, so each must have either illimited \( \mathcal{E} \), or non-nearstandardly concentrated density, or both. But since these non-nearstandard vectors enter \( \tilde{\Gamma} \) with a combined weight of at least \( \epsilon/2 \), \( \tilde{\Gamma} \) itself and a fortiori \( \Gamma \) must also have either illimited \( \mathcal{E} \) or non-nearstandardly concentrated density. But, that is contrary to hypothesis.

This Proposition has a couple of easy but important corollaries.

**Corollary 4.1.** If \( \rho \in X \) satisfies \( F(\rho) < \infty \), then there exists \( \gamma \in \mathcal{G} \) with \( \text{Dens} \gamma = \rho \) and \( E(\gamma) = F(\rho) \).

**Proof.** Since \( F(\rho) < \infty \), there is some \( \gamma \in \ast \mathcal{G} \) with \( \text{Dens} \gamma = \rho \) and \( E(\gamma) \approx F(\rho) \). By Prop. 4.1 \( \gamma \) is nearstandard. Then, since \( \mathcal{E} \) is lower semicontinuous, bu Lemma 4.2 \( \mathcal{E}(\ast \gamma) \leq F(\rho) \). Since both sides of this inequality are standard,
\[ \mathcal{E}(\ast \gamma) \leq F(\rho). \]
On the other hand, $Dens : \mathcal{S} \to X$ is continuous, which implies that $\rho$ is in the monad of $Dens \circ \gamma$. But, $\rho$ is standard, so $Dens \circ \gamma = \rho$. Therefore, $\mathcal{E}(\gamma) \geq F[\rho]$, which combined with the previous display yields $\mathcal{E}(\gamma) = F[\rho]$.

**Corollary 4.2.** Let $T$ be a topology on $Range Dens$ which makes the map $Dens$ from mixed-states to 4-densities continuous. then $F$ is lower semicontinuous with respect to $T$.

**Proof.** Let $\rho$ be a 4-density in $Range Dens$ and $\rho' \in Range Dens = Range *Dens$ such that $\rho' \approx \rho$. And, let $\gamma'$ be a *density matrix with $Dens \gamma' = \rho'$. By Prop. 4.1, $\gamma'$ is nearstandard. Thus, $Dens \circ \gamma'$ is a standard density which is infinitely close to $\rho'$ by the assumption of $Dens$. Therefore, $Dens \circ \gamma' = \rho' = \rho$, so that

$$F[\rho'] = \mathcal{E}_1(\gamma') \geq \mathcal{E}_1(\gamma) \geq F[\rho],$$

where the almost-inequality follows from Lemma 4.2 and the final inequality by definition of $F[\rho]$.

---

### 5. COARSE-GRAINING

This section reviews the basic notions of the coarse-grained DFT framework of References 20, 22, augmented to the SDFT setting. Much of it looks exactly the same on the surface as the conventional fine-grained theory of Sec. 2. Building on the results of Sec. 4, the existence and regularity results for the coarse-grained theory will be presented in Sec. 6. In addition to the considerably simpler and more intuitive proofs, these results go beyond the previous version of the theory by treating spin-densities.

Consider the partition $\mathcal{P}$ of $\mathbb{R}^3$ into a regular array of cubical cells $\Omega_\ell$ of side length $\ell$. A coarse-grained 4-density is simply a specification of the average 4-density in each cell. As such, a coarse-grained 4-density is an equivalence class of densities in $X$, the members of the class differing only in the way particle number and spin is distributed within the cells. Generally, coarse-grained densities are denoted by the same sorts of symbols as were used previously for fine-grained densities, but there should be no confusion as the rest of the paper focusses on coarse-grained densities. Since $\rho$ assigns an average density to a cell, it is convenient to identify $\rho$ with the leveled-out function which is equal to that average throughout the cell. That makes $\rho$ into a piecewise constant function. This is just a very convenient representation; the lack of smoothness has no real significance. What is done with the (shared) faces of the cubes does not matter since they have zero Lebesgue measure. The coarse-grained densities now belong to the $L^1$ space of cell-constant 4-component functions with norm

$$\|f\|_1 := \int_{\mathbb{R}^3} \left(|f_0(x)| + |f_1(x)|\right) dx. \quad (18)$$

This Banach space, which will be denoted $X$, is a subspace of $\mathcal{P}$, so we could also describe matters with the aid of the projection $\pi : X \to \mathcal{P}$ which averages over cells of $\mathcal{P}$. Then, we are identifying $\rho$ with $\pi \rho$, since $\pi \eta$ is the same for every $\eta \in \rho$.

Some useful subspaces of $X$ are singled out:

$$X^+ := \{\rho \in X : \rho \geq 0\}$$

$$X^{++} := \{\rho \in X^+ : \rho \geq \rho_0\} \quad (19)$$

$X^+$ consists of true densities, $X^{++}$ adds the restriction that the number-density does not vanish on any cell, which is a physically untroubling restriction, as presumably an infinite potential would be needed to drive the density to zero on an entire cell. If $|\rho| = \rho_0$ on some cell, that cell is said to be spin-saturated. Subspaces without spin saturation

$$X^\oplus := \{\rho \in X^+ : |\rho| < \rho_0\}$$

$$X^{\oplus\oplus} := \{\rho \in X^{++} : |\rho| < \rho_0\} \quad (20)$$

are also defined. Only $X^{\oplus\oplus}$ can be fully controlled in a general way, but collinear spin-saturated states will be treated in Sec. 8.

A fine-grained density in the conventional theory has associated with it a whole set of states, and some are selected out by an energetic criterion. We do the same here. The Lieb internal energy functional is defined as

$$F[\rho] := \inf \{\mathcal{E}(\Gamma) : \Gamma \in \mathcal{S}, \pi Dens \Gamma = \rho\}, \quad (21)$$

for $\rho$ in $X$, in perfect analogy to the conventional case. If there are no states with $\pi Dens \Gamma = \rho$, then $F[\rho] = +\infty$, as usual. But, there are states realizing any density in $X^+$, and

$$F[\rho] \leq \|\rho\|_1 V_0, \quad \text{for } \rho \in X^+, \quad (22)$$

where the constant $V_0$ depends on $\ell$. This is in stark contrast to the continuum situation, and arises because there is a finite intrinsic energy cost $N V_0$ to putting all the particles in the same cell of $\mathcal{P}$. Any density in $X^+$ can at least be realized by a mixed-state sum of such single-cell states, and the bound follows. Since for $t \in [0, 1]$, the convex combination $t \Gamma + (1-t)\Gamma'$ of density matrices gives the corresponding convex combination of densities, it is immediate that $F$ is convex:

$$F[t \rho + (1-t)\rho'] \leq t F[\rho] + (1-t)F[\rho']. \quad (23)$$

Now we turn to potentials. For $\rho \in X$, any cell-constant 4-vector function $v$ which is bounded below and satisfies

$$F[\rho'] + \langle v, \rho' \rangle \geq F[\rho] + \langle v, \rho \rangle = 0 \quad \forall \rho' \in X, \quad (24)$$

is called a representing potential for $\rho$. The reason for the name is clear: there is a state $\Gamma$ with $\pi Dens \Gamma = \rho$ with total energy 0 in presence of $v$, and no state with lower energy. The stipulation that the ground state energy be zero merely fixes the constant which could otherwise be
The argument work. The conclusion is correspondingly
restriction to a fixed finite volume allows us to make
courses, and coarse-grained theories. However, in the latter, a
ential principle that we will use is the product
topology. Neighborhoods correspond to constraints on
next section will show that all of $\mathcal{X}^{\oplus \oplus}$ is VREP.
Because the cells of $\Phi$ are non-infinite-only, there is a
state density of $\rho$ which is all that will be needed, is denoted $\mathcal{V}$. Necessarily,
Potl (\rho) \subset \mathcal{V}. Similarly, an upper bound can be obtained
if we also consider the density. If $v \in \text{Potl}(\rho)$, then it is easy to see that
\begin{equation}
(v_0 - |\vec{v}|)\rho_0 \leq N \frac{V_0}{F^1}.
\end{equation}
The only topology on $\mathcal{V}$ that we will use is the product
topology. Neighborhoods correspond to constraints on
the potential on a finite number of cells, and a basis is
given by sets of the form
\begin{equation}
U_{\epsilon,L}(w) = \{ v \in \mathcal{V} : |w - v| < \epsilon, \forall |x| < L \}
\end{equation}
parametrized by $\epsilon, L > 0$ and $w \in \mathcal{V}$, where $|w - v| = v_0 - v_0 + |\vec{v} - \vec{v}|$. Convergence of a sequence of potentials
with respect to the product topology is cell-wise convergence.

6. V-REPRESENTABILITY AND REGULARITY

This section is the core of the paper. In it, all the basic existence and regularity results are given. In the following section, the uniqueness question is taken up.

A. baby steps

In Sec. we noted that $\text{epi} F = \{(\rho^*, y) \in \mathcal{X} \times \mathbb{R} : y \geq F[\rho^*]\}$ is convex and closed, but despite that, a straightforward Hahn-Banach argument is not available to prove V-representability of even one density because $\text{dom} F$ has empty interior. This problem is common to the conventional and coarse-grained theories. However, in the latter, a restriction to a fixed finite volume allows us to make the argument work. The conclusion is correspondingly weaker, of course, but the simplified problem will serve as a foundation on which to build a solution to the general problem.

Consider the densities in $\mathcal{X}^+$ which are supported in the cube $\Lambda_L^+ (|x^i| \leq L$ for $i = 1, 2, 3$) and call this set $\mathcal{X}^+_L$. Then, $\mathcal{X}^+_L$ is a convex set with nonempty interior, viewed as a subset of $\mathbb{R}^{4L^3}$; this interior consists of densities which are strictly positive over $\Lambda_L$ and nowhere spin-saturated. The restriction of $F$ to $\mathcal{X}^+_L$ is a convex function with an upper bound given by inequality (22). In this case, all the conditions are satisfied to apply the separation theorem, and the boundedness of $F$ implies that a separating hyperplane at an interior point $\rho$ is not vertical. Thus, it can be represented as a potential $v$ in this restricted sense:
\begin{equation}
F[\rho^*] + \langle v, \rho \rangle \geq F[\rho^*] + \langle v, \rho \rangle = 0 \ \forall \rho^* \in \mathcal{X}^+_L.
\end{equation}
In this case, we say that $\rho$ is L-VREP. The nomenclature is meant to emphasize the property it has which is akin to V-representability, even though it is just equivalent to being supported essentially on $\Lambda_L$ but nowhere spin-saturated on that set.

B. hyperfinite bootstrap

Using the modest result of the previous subsection, we now launch into the hyperfinite. From there, the infinite volume limit is an easy step down. Since the L-VREP property is standard and holds for every $L \in \mathbb{N}$, it holds in the nonstandard extension for every $L \in \mathbb{N}$, by the Transfer Principle. This simple observation paves the way for the following key Lemma. The potentials which occur in the hypothesis are in $\text{ns}^* \mathcal{V}$, that is, in $\text{ns}^* \mathcal{V}$ and near-standard. Since $\mathcal{V}$ has the product topology, $v \in \text{ns} \mathcal{V}$ means that $|v| > -V_0$ and $\exists x$ is limited at all limited locations $x$.

Lemma 6.1. If $\rho \in \mathcal{X}$ is nearstandard, and is either
VREP or L-VREP for $L \approx +\infty$, with a representing potential $v \in \text{ns}^* \mathcal{V}$, then
(i). $\text{st} v \in \text{Potl}(\text{st} \rho)$
(ii). $F[\text{st} \rho] \approx F[\text{st} \rho]
(iii). $v \cdot \rho$ is nearstandard in $L^1$, hence $v \cdot \rho \approx v \cdot \rho$.

Proof. According to the hypothesis,
\begin{equation}
F[\rho] + \langle v, \rho \rangle = 0,
\end{equation}
for some $v \in \text{ns} \mathcal{V}$. We will show below that
\begin{equation}
F[\rho^*] + \langle v, \rho^* \rangle \geq 0, \ \forall \rho^* \in \mathcal{X}^+,
\end{equation}
and that
\begin{equation}
\langle v, \rho \rangle \lesssim \langle v, \rho \rangle.
\end{equation}
With $F[\rho^*] \lesssim F[\rho]$ from Cor. this yields $F[\rho^*] + \langle v, \rho \rangle \lesssim 0$. Since $F[\rho^*]$ and $\langle v, \rho \rangle$ are standard, all these near-inequalities imply
\begin{equation}
F[\rho] + \langle v, \rho \rangle = 0,
\end{equation}
as well as
\[ F[\delta \rho] \approx F[\rho], \quad \langle \delta v, \delta \rho \rangle \approx \langle v, \rho \rangle. \] (32)

This last display gives part \((ii)\), and \((i)\) together prove part \((i)\).

So, to fill in the gaps, suppose that \(\rho'\) violates condition \((i)\):
\[ F[\rho'] + \int_{\mathbb{R}^3} \delta v \cdot \delta \rho \, dx < 0. \] (33)

Then, there is a smooth truncation \(\rho''_R\) of \(\rho'\) that also violates condition \((i)\). (“Smooth truncation” here refers to the construction in Lemma \(6.1\), which is really applied to the state underlying \(\rho'\), not to the density itself.) For, by taking the truncation radius \(R\) big enough, \(F[\rho''_R]\) can be made as close as desired to \(F[\rho']\). At the same time,
\[ \int_{\mathbb{R}^3} \delta v \cdot \delta \rho \, dx = \int \langle \delta v \cdot \delta \rho \, dx \rangle - \int \langle \delta v \cdot \delta \rho \, dx \rangle, \]
and taking \(R\) large makes the change in the integral over the negative part as small as needed, due to condition \((i)\), while the integral over the positive part can only decrease, which is not a threat to the inequality.

Thus, \(\rho'\) in \((i)\) may be assumed to have bounded support. But in that case \(\langle \delta v \cdot \delta \rho \rangle \approx \langle v \cdot \rho' \rangle\), since both integrals are effectively only over the \(R\)-ball \(B_R\), and \(v\) is limited there, indeed uniformly bounded both above and below on \(B_R\). But then \(F[\rho'] + \langle v \cdot \rho' \rangle < 0\). This is contrary to the VREP hypothesis on \(\rho\) in case \(\rho\) is only L-VREP, the fact that \(\rho'\) has bounded support also enters the argument. Thus, condition \((i)\) is proven.

Similar reasoning using the lower bound on \(v\) and near-standard concentration of \(\rho\) proves inequality \((ii)\).

\((iii)\): Both \(\rho\) and \(v\) are limited at limited points. Thus, if \(v \cdot \rho\) is nearstandard in \(L^1\), then \(v \cdot \rho\) is its standard part. To show \(\rho \cdot v\) is nearstandard, it will suffice to verify that \(\int_{|x| > L} (v \cdot \rho) \, dx \approx 0\) for illimited \(L\). (The last few paragraphs of Sec. \(3\) are relevant to these considerations.)

Since \(\rho\) is nearstandard, the lower bound \(\rho(\mathbb{R}^3) \approx 0\). On the other hand, combining that with \(\int_{|x| > L} |(v \cdot \rho)| \, dx \approx 0\) and \(\langle v, \rho \rangle \approx \langle v, \rho \rangle\) yields \(\int_{|x| > L} (v \cdot \rho)^+ \, dx \approx 0\).

A general VREP result follows immediately. Recall the definition \(10\) of \(X^{\mathbb{R}^3}\).

**Proposition 6.1.** Every \(\rho \in X^{\mathbb{R}^3}\) is VREP.

**Proof.** Truncate \(*\rho\), by setting it to zero outside \(\Lambda_L\) for illimited \(L\). This density is L-VREP, and Lemma \(6.1\) then gives the result. \(\square\)

Now, by the Transfer Principle, all densities in \(*X^{\mathbb{R}^3}\) are VREP, so that Lemma \(6.1\) applies to any density in \(*X^{\mathbb{R}^3}\). This observation yields two additional corollaries.

**Proposition 6.2.** \(\rho \mapsto F[\rho]\) is continuous.

**Proof.** Take \(\rho\) a standard density and \(\rho' \approx \rho\). According to the transferred version of Prop. \(6.1\), \(\rho'\) is VREP, and by Lemma \(6.1\) \((ii)\), \(F[\rho'] \approx F[\rho]\). \(\square\)

The second corollary is about continuity-like properties of \(\text{Potl}\) as a function of density. Since \(\rho \mapsto \text{Potl}(\rho)\) is a set-valued map, we need to discuss what continuity means in that case. A set-valued map \(f : X \mapsto Y\) between topological spaces is said to be upper semicontinuous at \(x \in X\) if, for any open set \(U\) containing \(f(x)\), there is a neighborhood \(V\) of \(x\) such that \(f(z) \subseteq U\) for every \(z \in V\). Upper semicontinuity of \(\rho \mapsto \{v \cdot \rho : v \in \text{Potl}(\rho)\}\) will be shown to hold on \(X^{\mathbb{R}^3}\). This cannot hold on all of \(X\) because \(\text{Potl}\) takes the value \(\emptyset\) at some densities with \(\rho_0 = 0\) somewhere. However, we will show that the graph of \(\text{Potl}\) is closed in \(X \times V\). This means that if \((\rho_n, v_n)\) in Graph \(\text{Potl}\) is a sequence of density/potential pairs with \((\rho_n, v_n) \to (\rho, v) \in X\) in \(L^1\) and \(v_n \to v \in V\) cell-wise, then \(v \in \text{Potl}(\rho)\).

**Proposition 6.3.** \((a)\) For every \(\rho \in X\), \(\text{Potl}(\rho)\) is closed in product topology.

\((b)\) Graph \(\text{Potl}\) is closed in \(X \times V\).

\((c)\) The set-valued map \(\rho \mapsto \{v \cdot \rho : v \in \text{Potl}(\rho)\}\) is \(L^1\) upper semicontinuous on \(X^{\mathbb{R}^3}\).

**Proof.** Recall the nonstandard characterization of a closed set: \(A\) is closed if and only if all nearstandard points of \(*A\) are infinitely close to \(A\).

\((a)\) Let \(v \in *\text{Potl}(\rho)\) be nearstandard. Then \(v \in \text{Potl}(\rho)\).

\((b)\) Let \((\rho, v)\) be a nearstandard point in \(*\text{Graph Potl} = *\text{Graph Potl}\). This means that both \(\rho\) and \(v\) are nearstandard. By Lemma \(6.1(i)\), \(\langle \rho, v \rangle = \langle \rho, \rho \rangle \in \text{Graph Potl}\).

\((c)\) Let \(\rho \in *X^{\mathbb{R}^3}\) and \(v \in \text{Potl}(\rho)\) both be nearstandard. Then, \(\rho\) is VREP by the transferred version of Prop. \(6.1\). Thus, by Lemma \(6.1(iii)\), \(st (v, \rho)\) is infinitely close to some element of \(*\rho \cdot \text{Potl}(\rho)\). \(\square\)

Finally, we show that \(\text{Potl}\) is the functional derivative on \(X^{\mathbb{R}^3}\), in a sense appropriate to general convex functionals. Recall that for \(\rho, \rho + \delta \rho \in X^{\mathbb{R}^3}\), convexity of \(F\) guarantees existence of the directional derivative
\[ F'(\rho; \delta \rho) := \lim_{\epsilon \downarrow 0} \frac{1}{\epsilon} (F[\rho + \epsilon \delta \rho] - F[\rho]). \]

By the very definition of \(\text{Potl}(\rho)\),
\[ \langle -v, \delta \rho \rangle \leq F'(\rho; \delta \rho), \]
for every \(v \in \text{Potl}(\rho)\). What the next result says is that this inequality is saturated:
\[ F'[\rho; \delta \rho] = \max \{\langle -v, \delta \rho \rangle : v \in \text{Potl}(\rho)\}. \] (34)

Thus, all directional derivatives can be recovered from \(\text{Potl}(\rho)\). If \(\text{Potl}(\rho)\) is a singleton, it is easy to see that the
potential can be obtained from the directional derivatives in a local way:

$$v_i = \frac{\partial F}{\partial \rho_i}.$$ 

That this remains the case in the non-unique case will follow from Prop. 6.2.

**Proposition 6.4.** For $\rho$ and $\rho' = \rho + \delta \rho$ in $\mathcal{X}_0^\oplus$, there is $v \in \text{Potl} (\rho)$ satisfying

$$\langle -v, \delta \rho \rangle = F' [\rho; \delta \rho].$$

Thus,

$$F' [\rho; \delta \rho] = \max \{ \langle -v, \delta \rho \rangle : v \in \text{Potl} (\rho) \}.$$

**Proof.** Let $\epsilon > 0$ be an arbitrary infinitesimal. Then, since (one-sided) directional derivatives of $F$ exist,

$$F [\rho + \epsilon \delta \rho] - F [\rho] = \epsilon (F' [\rho; \delta \rho] + \eta),$$

where $\eta \approx 0$. Now, $\rho + \epsilon \delta \rho$ is VREP by Prop. 6.1 and Transfer, so let $v \in \text{Potl} (\rho + \epsilon \delta \rho)$. Then,

$$F [\rho + \epsilon \delta \rho] - \langle -v, -\epsilon \delta \rho \rangle \leq F [\rho].$$

Together with the previous displayed equation, this yields

$$\langle -v, \delta \rho \rangle \geq F' [\rho; \delta \rho].$$

(35)

On the other hand, by Lemma 6.1, $v \in \text{Potl} (\rho)$, implying that

$$\langle -\delta, \delta \rho \rangle \leq F' [\rho; \delta \rho].$$

(36)

We would like to get equality here by showing that the near-inequality is, roughly speaking, nearstandardly carried, in order to replace “$\leq$” in (35) with “$\geq$”.

Suppose then that this hope is dashed and

$$\int_{|x| > L} v \cdot \delta \rho \, dx \ll 0,$$

(37)

for some $L \approx \infty$. By the argument in Lemma 6.1

$$\int_{|x| > L} v \cdot (\rho + \epsilon \delta \rho) \, dx \approx 0,$$

otherwise truncation would show that $\rho + \epsilon \delta \rho$ is not the ground state density of $v$. But, then, by combining the last two displays,

$$\int_{|x| > L} v \cdot (\rho + \delta \rho) \, dx \ll 0.$$

(38)

Now, a “backward truncation” of $\rho + \delta \rho$, keeping just the part for $|x| > L$ would have infinitesimal intrinsic energy, but potential energy appreciably less than zero, again implying that $\rho + \epsilon \delta \rho$ is not a ground state density in $v$. Thus, (36) is false, implying that the inequality is nearstandardly carried and the inequality in (35) can be turned around. This proves the Proposition. 

### 7. Four-Potential Uniqueness and Non-Uniqueness

This section is concerned with the question of when $\text{Potl} (\rho)$ might have more than one element. This problem attracted renewed scrutiny in the conventional setting, long after the original investigation. The conclusion reached here (Prop. 7.2) is similar to the cumulative conclusion of those works. But here unique continuation properties are demonstrated rather than being assumed. In quick summary, disallowing spin-saturation leaves the only possibility of non-uniqueness being collinear magnetization in an $S_2$ eigenstate. The next section looks more closely at the collinear case with spin-saturation. No nonstandard analysis is used in either of these two sections.

In contrast to previous sections, it is necessary to carefully consider the behavior of wavefunctions in configuration space. Throughout this section, $\Psi$ is a fixed ground state wavefunction of total energy $0$ in the presence of potential $v = (u, \vec{B})$:

$$(H_0 + \hat{V})\Psi = 0,$$

(39)

where

$$\hat{V} = \sum_{\alpha=1}^N [u(x_\alpha) + \vec{B}(x_\alpha) \cdot \vec{\sigma}_\alpha].$$

(40)

Here, $H_0$ contains kinetic energy and interaction energy and is diagonal in spins. The potential at the position of particle $\alpha$ is $(u(x_\alpha), \vec{B}(x_\alpha))$. $\Psi$ might be a zero-energy ground state for some other potential. Elements of $\text{Potl} (\Psi)$ other than $(u, \vec{B})$ are generically denoted as $(u', \vec{B}')$. It will soon become clear that, in studying the non-uniqueness problem, only the magnetic field component really requires attention. To facilitate that, the notation

$$\text{Potl} (\rho) = \{ \vec{B} : (u, \vec{B}) \in \text{Potl} (\rho) \text{ for some } u \}$$

will be used for the projection of $\text{Potl} (\rho)$. Naturally extending previous notation, $\text{Potl} (\Psi)$, denotes the set of four-potentials having $\Psi$ as a zero-energy ground state. As previously, position space cells (“$\Psi$-cells”) are denoted $\Omega_i$, etc., $i$ being simply an abstract cell index. Cells in configuration space (“$\Psi^N$-cells”) are denoted in the style $\Omega_{11\cdots i\cdots N}$. In cell $\Omega_{11\cdots i\cdots N}$, particle 1 is in $\Omega_i$, ..., particle $N$ is in $\Omega_N$. The value of $(u, \vec{B})$ in cell $\Omega_i$ is denoted $(u_i, \vec{B}_i)$. In this section and the next, instead of $(\rho_0, \vec{B}_0)$ for the 4-density $\tau \text{Dens} \Psi$, we use the notation $\{n_i, 2m_i\}$ (Note the factor of 2). If for every $(u', \vec{B}') \in \text{Potl} (\Psi)$, $\vec{B}' = \vec{B}_i$, then $i$ is a unique-\$B cell (UB cell), otherwise a non-unique-\$B cell (non-UB cell).

The following unique continuation result for single-component wavefunctions is fundamental.
Thm. XIII.63 of RSIV. Let $u \in H^2_{\text{loc}}$, that is, $\phi u \in D(-\Delta)$ for each $\phi \in C_0^\infty(\mathbb{R}^n)$. Let $D$ be an open connected set in $\mathbb{R}^n$ and suppose that

$$|\nabla^2 u(x)| \leq M|u(x)|$$  \hspace{1cm} (42)

almost everywhere in $D$. Then, if $u$ vanishes in the neighborhood of a single point $x_0 \in D$, $u$ is identically zero in $D$.

$M$ is supposed to be an arbitrary but fixed constant. An examination of the proof of the basic unique continuation theorem shows that it extends to multicomponent wavefunctions, such as wavefunctions with spin indices, by replacing $|u|^2$ and $|\nabla^2 u|^2$ by the corresponding sums of squares of spin components. Indeed, this replacement can simply be made globally throughout the proof of the theorem and lemmas leading up to it. Unfortunately, that does not immediately give us any control of individual spin components. The usual way a bound of the sort (42) arises, of course, is that $u$ satisfies a Schrödinger equation, so that $M = |V - E|$. An individual spin component might satisfy such an equation by itself. If it is appropriately related to a different component that does so, that can also work.

It may appear at first that the unboundedness of the Coulomb repulsion could cause problems. On any $\Lambda_L$, the single-particle external potential is bounded, so the total external potential is bounded on $\Lambda_L^N$. The sum of the external potential and the interaction is then uniformly bounded on $U_{L,n} = \Lambda_L^N \cap U_n$ for any $n$, where $U_n = \{ x : |x_i - x_j| > 1/n, \forall i \neq j \}$. Also, $U_{L,n}$ is a connected (open) set for large enough $n$, so the theorem will apply to it. But, any open subset of $\Lambda_L^N$ must have an open intersection with $U_{L,n}$ for some $n$. So, in fact, we are free to take $D$ to be $\Lambda_L^N$. This depends on the set where the interaction energy is infinite having small codimension and no interior. Our first application of the theorem is then to note that if $\Psi \equiv 0$ on any $\Omega_{i_1 \cdots i_N}$, then it vanishes everywhere. Thus, there is nonzero probability to be in any $\Psi^N$-cell.

Note in passing that, by basic elliptic regularity theory, $\Psi$ is continuous away from coincident configuration points $(x_\alpha = x_\beta$ for $\alpha \neq \beta)$ and is $C^\infty$ away from coincidence on the boundaries of the $\Psi$-cells.

If $(u', \vec{B}') \in \text{Potl}(\Psi)$ is distinct from $(u, \vec{B})$ then with $\Delta u = u' - u$ and $\Delta \vec{B} = \vec{B}' - \vec{B}$,

$$\Delta \hat{V} \Psi = \sum_{\alpha=1}^N \left[ \Delta u(x_\alpha) + \Delta B(x_\alpha) \cdot \vec{\sigma}_\alpha \right] \Psi = 0.$$  \hspace{1cm} (43)

It then follows that $[H_0 + \hat{V}, \Delta \hat{V}] \Psi = 0$. As a distributional equation on the interior of the configuration space cell $\Omega_{i_1 \cdots i_N}$ this yields

$$\sum_{\alpha=1}^N (\vec{B}_{i_\alpha} \times \Delta \vec{B}_{i_\alpha}) \cdot \vec{\sigma}_\alpha \Psi = 0.$$  

Now take the commutator of $H_0 + \hat{V}$ with the new operator, to find

$$\sum_{\alpha=1}^N (\vec{B}_{i_\alpha} \times (\vec{B}_{i_\alpha} \times \Delta \vec{B}_{i_\alpha})) \cdot \vec{\sigma}_\alpha \Psi = 0.$$  

These equations are useful in the case of $\Omega_{i_1 \cdots i_N}$. Our basic unique continuation result assures that $\Psi$ does not vanish on any open set in this cell, so the equations are not vacuous.

First, note from Eq. (43) that if $\Delta \vec{B}_i = 0$, then $\Delta u_i = 0$ as well. So a UB cell also has unique $u$, explaining the focus on the UB/non-UB dichotomy. Thus, suppose that $\Omega_i$ is a non-UB cell. Then, $\Delta \vec{B}_i$ can be taken nonzero, and so can $\vec{B}_i$ (otherwise flip the roles of $\vec{B}_i$ and $\vec{B}'_i$). If $\Delta \vec{B}_i$ is not parallel to $\vec{B}_i$, that makes $\Psi$ an eigenstate of spin along two perpendicular axes, which is impossible. Thus, $\Delta \vec{B}_i$ is parallel to $\vec{B}_i$.

**Lemma 7.1.** If $\Omega_i$ is a non-UB cell, then there is a unique axis $\hat{e}_i$, such that for every $\vec{B}$ in $\text{Potl}(\Psi)$, $\vec{B}_i$ is parallel to $\hat{e}_i$, that is, $\vec{B}_i = B_i \hat{e}_i$.

**Proof.** See previous paragraph. \hfill $\square$

If $\Omega_j$ is a UB cell with $\vec{B}_j \neq 0$, there is also a unique axis $\hat{e}_j$, namely $\vec{B}/|\vec{B}|$. If $\vec{B}_j = 0$ is unique, $\hat{e}_j$ is arbitrary. Each cell $\Omega_j$ thus has its own spin quantization axis $\hat{e}_j$. In the following, we will mostly use this $\hat{e}_j$-basis. That is, in $\Omega_{i_1 \cdots i_N}$, the component $\Psi_{s_1 \cdots s_N} = (s_1 \cdots s_N) \Psi$ has the spin of particle $\alpha$ up along $\hat{e}_{\alpha}$, if $s_\alpha = +1$ and down along $\hat{e}_{\alpha}$, if $s_\alpha = -1$.

Consider now the restriction of $\Psi$ to $\Omega_{i_1 \cdots i_N}$. The external four-potential is diagonalized in the $\hat{e}$ basis, so the unique continuation theorem quoted above can be applied separately to each component $\Psi_{s_1 \cdots s_N}$ to see that if $\Psi_{s_1 \cdots s_N}$ vanishes on any open set in $\Omega_{i_1 \cdots i_N}$, it vanishes almost everywhere on the cell $\Omega_{i_1 \cdots i_N}$.

At this point, we want to consider $\Omega_{i_1 \cdots i_{k+1} \cdots i_N}$ with $i_{k+1}, \ldots, i_N$ all different from $j$.

**Lemma 7.2.** If $\Omega_j$ is non-UB, then, for fixed $\Omega_{j_{k+1} \cdots i_{k+1} \cdots i_N}$ with $i_{k+1}, \ldots, i_N$ all different from $j$, the $s_{k+1} \cdots s_N$ component of $\Psi$ (in $\hat{e}$ basis) is an eigenstate of spin along $\hat{e}_j$. That is, for only one $s_1, \ldots, s_k$ is $\Psi_{s_1 \cdots s_N}$ nonzero.

**Proof.** This follows straightforwardly from the eigenfunction Eq. (43). $\Delta B_j$ can be assumed to be nonzero along $\hat{e}_j$, giving

$$k \Delta u_j + \Delta B_j (k - 2N_j) + \sum_{\alpha=k+1}^N (\Delta u_{i_\alpha} + \Delta B_{i_\alpha}, s_\alpha) = 0,$$

where $N_{j_k}$ is the number of spin-down particles in $\Omega_j$. The equation has at most one solution for $N_{j_k}$.

**Proposition 7.1.** If $\Omega_j$ is a non-UB cell, then $\hat{e}_j \times \vec{m}_j = 0$.\hfill $\square$
Proof. This follows from Lemma 7.2 by summation over cell occupations and integration.

At this point we turn attention from a single configuration space cell to a pair of neighboring cells $\Omega_{i_2\cdots i_N}$ and $\Omega_{j_2\cdots j_N}$; “neighboring” means that $\Omega$ shares a face with $\Omega_j$. The indices $i_2 \cdots i_N$ are fairly inert, so the cell index notation is abbreviated to $\Omega_{i[k]}$ and $\Omega_{j[k]}$.

For the following argument we use a slight modification of the $\hat{e}$ basis, namely using $\hat{e}_k$ in both $\Omega_k$ and $\Omega_j$, $(\hat{e}_k[i] \cdot \hat{e}_k[j])$-basis).

**Lemma 7.3.** Suppose that $\Omega_j$ and $\Omega_k$ are neighboring cells. Using $\hat{e}_k[i] \cdot \hat{e}_k[j]$-basis in both $\Omega_{j[i]}$ and $\Omega_{k[i]}$, if $\Psi_{s_1 \cdots s_N}$ vanishes in $\Omega_{j[i]}$, then it also vanishes on $\Omega_{k[i]}$.

Proof. The unique continuation theorem is applicable because the potential is diagonalized in $\Omega_{i[k]}$, while the condition (12) for our chosen component is satisfied in $\Omega_{j[i]}$, by hypothesis.

A possibly useful mnemonic is to say that “moving one particle from one cell to another cannot flip the spins of other particles”, bearing in mind that “moving” does not refer to a dynamical process but just a shift of attention.

**Lemma 7.4.** If $\Omega_j$ and $\Omega_k$ are neighboring $\Psi$-cells and both non-UB, then $\hat{e}_j$ and $\hat{e}_k$ are parallel.

Proof. In the $\hat{e}$ spin basis, find an occupied $s[t]$ spin state in $\Omega_{j[i]}$, with all of $i_2, \ldots, i_N$ different from $j$ and $k$. Then $(-s)[t]$ is unoccupied by Lemma 7.2. Also, there is some occupied $s'[t]$ in $\Omega_{k[i]}$, in $\hat{e}_k[i]$-basis. For if there were no such $s'$, then Lemma 7.2 would guarantee that $s[t]$ is unoccupied in $\Omega_{j[i]}$. Furthermore, $(s'[t])$ is then unoccupied in $\Omega_{k[i]}$, again by Lemma 7.2.

Thus, in $\Omega_{k[i]}$,

$$\Psi(-s)[t] = (-s)[s']\Psi_{s'[t]} + (-s) - s'[t]\Psi(-s')[t] = (-s)[s']\Psi_{s'[t]}.$$ 

$\Psi(-s)[t] = 0$ in $\Omega_{k[i]}$, and therefore satisfies a bound of type (12) there. But, it also satisfies such a bound in $\Omega_{i[k]}$. This follows because $\Psi_{s'[t]}$ satisfies such a bound there by virtue of obeying a Schrödinger equation, and $\Psi(-s)[t]$ has a fixed proportionality to $\Psi_{s'[t]}$ in $\Omega_{i[k]}$ according to the previous display.

The basic unique continuation theorem then says that $\Psi(-s)[t] = 0$ in $\Omega_{i[k]}$. But that implies that $|s| = |s'|$, and since these spin states are eigenstates of $\hat{e}_j \cdot \hat{\sigma}$ and $\hat{e}_k \cdot \hat{\sigma}$ respectively, $\hat{e}_j$ and $\hat{e}_k$ are coaxial.

The picture according to what has been proven so far is of connected components of non-UB cells, separated by UB cells. On each connected cluster, there is a unique common $\hat{e}$ axis. So, it is now time to consider UB cells. It turns out that the existence of one has drastic consequences.

**Lemma 7.5. If there is a UB cell, then all non-UB cells are spin-saturated.**

Proof. Label one of the unique-$\vec{B}$ cells ‘0’. Then, considering the $\Psi^N$-cell $\Omega^N_{0\cdots 0}$ with all particles in $\Omega_0$, the eigenfunction Eq. (43) becomes $N\Delta u_0 = 0$. So, $\Delta u_0 = 0$ also.

Let $\Omega_j$ be a non-UB cell and look in $\Omega^N_{j\cdots 0}$. (If there are no non-UB cells, the Lemma is vacuously true.) The argument now is like that in Lemma 7.2.

$$\Delta u_j + \Delta \vec{B}_j \cdot \vec{\sigma}_1 = 0$$

for any spin component which occurs in the wavefunction in $\Omega^N_{j\cdots 0}$, where $\Delta \vec{B}_j$ can be taken non-zero along $\hat{e}_j$. This equation can be satisfied for only one value of $s_j = \hat{e}_j \cdot \vec{\sigma}$, either $+1$ or $-1$ but not both. Furthermore, $\Delta u_j = -s_j|\Delta \vec{B}_j|$. Shifting attention to $\Omega^N_{j\cdots 0}$, ..., $\Omega^N_{j\cdots k}$ in turn, the same argument shows that all the spins in $\Omega_j$ are in the $s^j$ spin state.

But, this argument does not tell us anything about the wavefunction in $\Omega^N_{0\cdots 0}$, where $\Omega_j$ and $\Omega_k$ are two different non-UB cells. If $|\Delta \vec{B}_j| = |\Delta \vec{B}_k|$, it looks as though it might be possible to flip a spin in each cell while continuing to respect Eq. (43).

Lemma 7.3 comes to the rescue here. For example, $\Omega^N_{j\cdots k}$ is saturated, by the preceding argument, and $\Omega^N_{j\cdots j}$ can be reached by moving (shift of attention) particle $N$ from one cell to another until $k$ is reached.

According to Lemma 7.3 at no step in this process do we see flips of the particles left in $\Omega_j$, so that the only possibility allowed by the eigenfunction Eq. (43) is that particle $N$ ends up in state $s^k$. It is clear how the example generalizes.

Thus, if there is even one unique-$\vec{B}$ cell, then any particle which is ever in the non-UB cell $\Omega_j$, is in spin state $s^j$. That shows spin saturation in cell $j$, namely, $|\vec{m}_j| = n_j/2$.

From the foregoing results, the main conclusion of this section can now be assembled. If there are UB ($\vec{B}$) cells as well as non-UB cells, then the latter are spin-saturated. We reconsider spin saturated cases in the next section, but for now assume no spin saturation, so this case is ruled out. All cells are thus non-UB, and all $\hat{e}_j$ are therefore along the same axis by Lemma 7.4. In that case, there is a global spin quantization axis which diagonalizes the Hamiltonian. $S_z$, the total spin along the common axis, is a good quantum number. Taking $\Psi$ to be an eigenstate of $S_z$, and looking at $\Omega_{ii\cdots i}$, we see that $\Delta u_i = -(2S_z/N)\Delta B_i$. Thus, different $S_z$ eigenstates cannot share more than one potential. Also, using this, the eigenfunction Eq. (43) becomes

$$\sum \Delta B_\alpha \left(-\frac{2S_z}{N} + \alpha \right) = 0,$$

which implies that all $\Delta B_\alpha$ are equal. Therefore,
Proposition 7.2. if \( \rho \) is nowhere spin-saturated but Potl(\( \rho \)) is not a singleton, then \( \vec{m} \) is everywhere along a common axis, \( \vec{m} = \bar{m} \hat{e} \), and the total spin \( \int m \, dz = S_z \) is a half-integer. Furthermore Potl(\( \rho \)) is a one-parameter family with \( \Delta \vec{B} \) only to be uniform:

\[
   u_i = u_i^0 - 2S_z \Delta B/N, \quad \vec{B}_i = \hat{e}[B_i^0 + \Delta B].
\]

Proof. Preceding discussion.

Note that this last result implies that Potl(\( \rho \)) can be locally determined from directional derivatives for variation of the density in only a single cell since such variations can be used to determine the ranges of \( u_i \) and \( \vec{B}_i \) and the proposition shows how to put them together to construct all of Potl(\( \rho \)).

8. COLLINEAR STATES AND SPIN-SATURATION

This short section takes up densities which are somewhere spin-saturated, especially the important case of collinear spin density. As for the general case, it is easy to see that a spin-saturated cell is non-UB, so according to the remark following Lemma 7.3 the saturated cells form clusters all magnetized in the same direction separated by non-spin-saturated, non-UB cells. Prop 6.3 (b) offers a possible route to find representing potentials for such densities.

The rest of this section concentrates on the collinear case. Thus \( \vec{m} \) is everywhere along the \( z \) axis, though it might be zero. Spin saturation has not been allowed in the general results of the previous two Sections, but collinear spin-saturated states clearly exist in nature, so it is important to make special provision for them.

Proposition 8.1. If \( \vec{m} \) is everywhere along the \( z \) axis, then so is \( \vec{B} \) for any \( \vec{B} \in \text{Potl}(\rho) \).

Proof. Assume \( \pi \text{Dens}\Psi = (n, 2m\hat{z}) \) with \( \vec{m} \) everywhere along \( \hat{z} \), and \( (u, \vec{B}) \in \text{Potl}(n, 2m\hat{z}) \). Simultaneous rotation of the spins and of \( \vec{B} \) by the same angle about the \( z \) axis preserves those relationships, as well as \( E(\Psi) \). Since \( \vec{m} \) is invariant under the rotation, if \( \vec{B} \bar{z} \) is not, then \( \Omega_z \) is a non-UB cell. But in that case, \( \vec{B} \bar{z} \) according to Prop. 7.1.

Proposition 8.2. If \( \rho = (n, 2m\hat{z}) \in X^{++} \) and \( \vec{m} \) is everywhere along the \( z \) axis, then Potl(\( \rho \)) \( \neq \emptyset \) if and only if \( \rho \) is either everywhere spin-saturated or nowhere spin-saturated.

Proof. The case of nowhere spin-saturated \( \rho \) has already been dealt with, so suppose that \( \rho \) is everywhere spin-saturated with \( \vec{m} = -2/n/2 \).

In the spinless version of the theory of Sec. 6, \( n = \rho_0 \) is V-representable; it is the density of some ground state \( \gamma \) in potential \( v \). Now, consider the family of four-potentials with \( \vec{B} = B\hat{z} \), and \( u - B = v \). The product of \( \gamma \) and [\( S_z = -N/2 \)] is an eigenstate of any of these \( v \). Since \( S_z \) is a good quantum number, all that needs to be done is to add a large enough uniform constant to \( B \) (and subtract it from \( u \)) so that the ground states in all other \( S_z \) sectors have greater energy than does \( \gamma \otimes [S_z = -N/2] \).

To see that other cases are not V-representable, assume \( \vec{m} = m\hat{z} \) with \( m = -n/2 \) somewhere, but not everywhere, so that \( (u, \vec{B}) \in \text{Potl}(\rho) \) satisfies \( \vec{B} = B\hat{z} \) according to Prop. 8.1. \( S_z \) is a good quantum number, so consider the ground state energies in each \( S_z \) sector. If \( S_z = -N/2 \) is not tied for minimum energy, the assumed situation is impossible. If a degeneracy does occur, then the \( S_z = -N/2 \) components can be removed from the state and the result is still a ground state for \( (u, \vec{B}) \). But this state has zero density in at least one cell, and that is impossible because it violates our basic unique continuation principle.

9. CONCLUDING REMARKS

This paper extends previously established results of coarse-grained DFT to SDFT. Here is a quick summary. As a function of coarse-grained four-density with \( L^1 \) norm, the Lieb internal energy functional \( F \) is continuous. For a coarse-grained density \( \rho \), the set of representing four-potentials which are constant on cells with additive constant fixed by \( F[\rho] + \langle v, \rho \rangle \) is a non-UB cell. Each four-potential \( v \) in Potl(\( \rho \)) has a ground state \( \gamma \) with a four-density that coarse-grains to \( \rho : \pi \text{Dens}\gamma = \rho \). If \( \rho \) is everywhere nonzero and nowhere spin-saturated \((\rho \in X^{++})\), then \( \rho \) is VREP: Potl(\( \rho \)) \( \neq \emptyset \). In fact, Potl is the functional derivative of \( F \) in this sense: for \( \rho \) and \( \delta \rho \) in \( X^{++} \), the directional derivative \( F'[\rho; \delta \rho] \) is equal to \( \langle -v, \delta \rho \rangle \) for all \( \rho \in \text{Potl}(\rho) \). Furthermore, if \( \rho \rightarrow \langle v, \delta \rho \rangle \) is an \( L^1 \) upper semicontinuous set-valued function, Potl takes values in closed sets and Graph Potl is closed in \( X \times V \). Apart from spin-saturated densities, only for densities \( \rho \) with collinear magnetization that integrates to a half-integer can Potl(\( \rho \)) have more than one element. And in that case, there is a global axis \( \hat{e} \) such that \( \vec{B} \) is everywhere along \( \hat{e} \) for all \( \vec{B} \in \text{Potl}(\rho) \) and different elements of Potl(\( \rho \)) differ by a uniform shift along \( \hat{e} \). Collinear states with fully saturated spin are also V-representable.

This paper has an additional aim of promoting the use of nonstandard analysis in mathematical and theoretical physics. The results of Section 6 were obtained with the aid of nonstandard analysis tools, resulting in proofs which are intuitive and of modest technical sophistication. The turn to infinitesimal methods was spurred by the hope that it would shed light on the limit of coarse-graining scale going to zero. In the meantime, it has shown its value for the infinite-volume limit.
ACKNOWLEDGMENTS

I thank Carsten Ullrich for a stimulating conversation at the 2009 APS March Meeting and Vin Crespi for suggestions on the manuscript.

1P. Parr and W. Yang, Density-Functional Theory of Atoms and Molecules (Clarendon, Cambridge, 1989).
2R. M. Dreizler and E. K. U. Gross, Density Functional Theory: an approach to the quantum many-body problem (Springer-Verlag, Berlin, 1990).
3H. Eschrig, The Fundamentals of Density Functional Theory (Teubner, Stuttgart, Leipzig, 1996).
4W. Koch and M. C. Holthausen, A Chemist’s Guide to Density Functional Theory, 2nd ed. (Wiley-VCH, Weinheim, 2001).
5R. van Leeuwen, in Advances in Quantum Chemistry, Vol. 43, edited by S. J. R. and B. E. (Elsevier, Amsterdam, 2003) pp. 25–94.
6A Primer in Density Functional Theory, edited by C. Fiolhais, F. Nogueira, and M. Marques, Lecture Notes in Physics, Vol. 620 (Springer-Verlag, Berlin, Heidelberg, 2003).
7E. Engel and R. M. Dreizler, Density Functional Theory An Advanced Course (Springer-Verlag, Berlin, Heidelberg, 2011).
8K. Capelle, Braz. J. Phys. 36, 1318 (2006), arXiv:cond-mat/0211443.
9M. Levy, Proc Natl Acad Sci USA 76, 6062 (1979).
10M. Levy, Phys. Rev. A 26, 1200 (1982).
11E. H. Lieb, Int J Quantum Chem 24, 243 (1983).
12H. Englisch and R. Englisch, Physica A 121, 253 (1983).
13P. Hohenberg and W. Kohn, Physical Review 136, B864 (1964).
14U. Von Barth and L. Hedin, J. Phys. C: Solid State Phys. 5, 1629 (1972).
15K. Capelle and G. Vignale, Solid State Comm. 118, 123 (2001).
16H. Eschrig and W. E. Pickett, Solid State Comm. 118, 123 (2001).
17C. A. Ullrich, Phys. Rev. B 72, 073102 (2005).
18N. I. Gidopoulos, Phys. Rev. B 75, 134408 (2007).
19J. T. Chayes, L. Chayes, and M. B. Ruskai, J. Stat. Phys. 38, 497 (1985).
20P. E. Lammert, J. Chem. Phys. 125, 074114 (2006).
21P. E. Lammert, Phys. Rev. A 82, 012109 (2010).
22P. E. Lammert, ArXiv:0908.1263v3.
23A. Robinson, Non-standard Analysis (North-Holland, Amsterdam, 1966) reissued by Princeton University Press, 1996.
24T. Lindstrom, in Nonstandard Analysis, edited by N. Cutland (Cambridge University Press, Cambridge, New York, 1988) pp. 1–105.
25R. Goldblatt, Lectures on the Hyperreals: an introduction to nonstandard analysis (Springer, New York, 1998).
26P. A. Loeb and A. E. Hurd, An introduction to nonstandard real analysis (Academic Press, Orlando, 1985).
27P. A. Loeb, in Nonstandard Analysis for the Working Mathematician, edited by P. A. Loeb and M. P. A. Wolff (Kluwer Academic Publishers, Dordrecht, Boston, 2000).
28M. Davis, Applied Nonstandard Analysis (Wiley, New York, 1977).
29N. I. Gidopoulos, Phys. Rev. B 75, 134408 (2007).
30P. Hohenberg and W. Kohn, Physical Review 136, B864 (1964).
31E. H. Lieb and M. Loss, Analysis (American Mathematical Society, Providence, R.I., 1997).