Consider a finite number of identical particles, fermions for instance. Let $a_i$ and $a_i^\dagger$ be their creation and annihilation operators at position $r$. Their number operator reads, $A = \int dr a_i^\dagger a_i$. Consider now a nuclear or atomic Hamiltonian, $H = T + V + U$, where $A, T = \sum_i t_i, V = \sum_{i>j} v_{ij}$ and $U = \sum_i u_i$ are the particle number, kinetic energy, two-body interaction energy and one-body potential energy, respectively. It is understood in the following that $u$ is local, $\langle r | u(r') = u(r) \delta(r - r')$, although generalizations of the theory to non local potentials are available. It is also understood that $u$ is a scalar, like $t$ and $v$, although non scalar $u$’s will be reinstated at the end of this note.

There is some frustration expressed in the literature at a contradiction between the existence theorem provided by Hohenberg and Kohn (HK), which deals with exact ground states having good quantum numbers, and the results given by those functionals used in practice, which often provide solutions showing spontaneously broken symmetries. The difficulty with such practical functionals comes, obviously, from their close connection with mean field theories, such as, for instance the Hartee-Fock (HF) variational principle. Moreover, the Kohn-Sham (KS) theorem, uses, orthogonal orbitals of independent particles, although its driving mean field does include, in principle, all the influence of correlations in a complicated wave function.

That mean field approximations lead to broken symmetries is actually a very good feature; there is no doubt indeed, for instance, that Ne$^{20}$ is a strongly deformed nucleus! But the subsequent projection of a good angular momentum is mandatory; indeed the ground state of Ne$^{20}$ is a $0^+$ and the relevant density is spherical, not prolate.

This note proves an existence theorem for a functional that allows simultaneously for mean fields breaking symmetries and for densities reflecting symmetry restoration. For the sake of generality, we can follow Mermin and use a finite temperature formalism. In Fock space, with a grand canonical ensemble, this means using the second quantized forms of $A$ and $H$, naturally. We first consider the domain $D$ of all density matrices $D$ in Fock space, under the obvious normalization constraint of a unit trace. Any approximation such as Hartee-Bogoliubov, BCS, shell model mixtures, generator coordinate mixtures, finite temperature HF, etc. then makes a restriction $\mathcal{R}$ of the domain $D$.

The usual variational principle, with a temperature $T$ and a chemical potential $\mu$, reads,

$$F_M = \min_{D \in \mathcal{D}} F,$$

$$F = \frac{\text{Tr} \, D (H - \mu A + T \ln D)}{\text{Tr} \, D}.$$  \hspace{1cm} (1)

With unrestricted density operators, it selects the well known, unique position, $D_M = \exp \left[ - (H - \mu A) / T \right] / Z$, where a smooth minimum, $F_M$, is reached. Any variation $\delta D$ away from $D_M$ creates a strictly positive increase of $F$ at second order with respect to $\delta D$. The functional double derivative, $\delta^2 F / \delta D \delta D'$, is strictly positive definite at that position $D_M$ in $D$. Accordingly, in any, whether local or global, system of coordinates for $D$, the matrix representing $\delta^2 F / \delta D \delta D'$ will be invertible.

From the very definition of $D_M$, the first order functional derivative, $\delta F / \delta D$, vanishes at that position. Hence, if one introduces an infinitesimal variation $\delta u$, triggering an infinitesimal displacement of $D_M$, the only contribution to $\delta F_M$ comes from $\delta u$. In short, $\delta F_M = \text{Tr} \, \delta D_M \, \delta U$. There is no contribution from $\delta D_M$.

Define the one-body density matrix in coordinate representation, $\nu(r, r') = \text{Tr} \, D_M a_i^\dagger a_{i'}$. Its diagonal, $\rho(r) = \nu(r, r)$, is the usual density deduced from $D_M$ by integrating out all particles but one. Hence $\int dr \, \rho(r) = \text{Tr} \, D_M \, A$. Note also the result, $\delta F_M = \int dr \, \rho(r) \, \delta u(r)$. In other words, $\delta F_M / \delta u = \rho$.

Freeze $t$ and $v$ and consider $F_M$ as a functional of $u$ alone. The Hohenberg-Kohn-Mermin (HKM) process then consists in a Legendre transform of $F_M$, based upon the essential result,

$$\frac{\delta F_M}{\delta u} = \rho.$$  \hspace{1cm} (2)

This Legendre transform involves two steps, namely i) subtract from $F_M$ the functional product of $u$ and $\delta F_M / \delta u$, namely the integral, $\int dr \, u(r) \, \rho(r)$, leaving

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$$F_M = \text{Tr} \, D_M \left( T + V - \mu A + T \ln D_M \right),$$  \hspace{1cm} (3)
then ii) consider \( \rho \) as the primary “variable” rather than \( u \), namely consider \( F_M \) as a functional of \( \rho \). Step ii) is made possible by the one-to-one correspondence between \( u \) and \( \rho \), under precautions such as the exclusion of those trivial variations \( \delta u \) which modify \( u \) by a constant only. (For some discussion of more precautions, see for instance [2] and [3].) The one-to-one correspondence is proven by an argument \textit{ab absurdo}: if distinct potentials \( u \) and \( u' \), generated (distinct!) \( D_M \) and \( D'_M \) with the same \( \rho \), then two contradictory, strict inequalities would occur, namely,

\[
\int dr [u(r) - u'(r)] \rho(r) < F_M - F'_M \quad \text{and} \quad \int dr [u(r) - u'(r)] \rho(r) > F_M - F'_M.
\]

(4)

An inverse Legendre transform, returning from \( F_M \) to \( F_M' \), is then available, according to the property,

\[
\frac{\delta F_M}{\delta \rho} = -u.
\]

(5)

Now, the \textit{same} properties and process hold if we assume that, when \( D \) is restricted to a smaller domain \( R \), there is still a \textit{unique} position \( D_m \) for a \textit{smooth again}, strict minimum, \( F_m = \operatorname{Min}_{D \in R} F \). The subscript \( M \) should be replaced by the subscript \( m \), but otherwise, it is trivial to recover Eq. (2) and the contradiction (4) to implement a one-to-one correspondence and a Legendre transform.

This will be illustrated by the special case of angular momentum restoration, at zero temperature. Limits at \( T = 0 \) are easy and do not need much discussion. Consider therefore a canonical situation, where is no need for \( \mu \); there is a well defined particle number \( A \), and density operators are dyadics, \( D = |\psi\rangle\langle\psi| \), where \( |\psi\rangle \) is just an \( A \)-particle wave function. The variational principle, Eq. (1), trivially reduces to the Rayleigh-Ritz form,

\[
F_M = \operatorname{Min}_\psi F, \quad F = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle},
\]

(6)

and the minimum with unrestricted wave functions generates the exact ground state with its exact eigenvalue \( F_M \), parametrized by \( u \). Restrict now the wave functions to be angular momentum projected Slater determinants,

\[
\Psi_0 = \int d\Omega R(\Omega) |\phi\rangle,
\]

(7)

where \( \Omega \) and \( R \) label rotation angles and rotation operators, respectively, and \( |\phi\rangle \) is an unrestricted, hence most often deformed, Slater determinant. Angular momentum \( 0 \) has been chosen here because every even-even nucleus has such a ground state. In a short, transparent notation, \( |\Psi_0\rangle = P_0 |\phi\rangle \), where \( P_0 \) can be normalized to be idempotent, \( P_0^2 = P_0 \). It commutes with \( H \), a scalar, and we use these commutation and idempotence in the following.

The key question is now whether there is a unique \( \Psi_{0m} \) for which the minimum,

\[
F_m = \operatorname{Min}_{\Psi_0} \frac{\langle\Psi_0|H|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle},
\]

(8)

is reached. Notice that, in any case, the restriction of trial functions enforces an inequality, \( F_m \geq F_M \), and that this inequality is generally strict, \( F_m > F_M \); it demands very special Hamiltonians and potentials for an equality to occur.

For deformed nuclei the same minimum \( F_m \), which also reads,

\[
F_m = \operatorname{Min}_\phi \frac{\langle\phi|H P_0|\phi\rangle}{\langle\phi|P_0|\phi\rangle},
\]

(9)

occurs for many choices of \( \phi \). All such Slater determinants are deduced from one another by rotations. Hence they generate the same projected state \( \Psi_0 \). As illustrated by Figure 1, that breach of uniqueness, namely the rotational degeneracy, caused at the \( \phi \) level by deformation, is completely corrected at the \( \Psi_0 \) level. There might be further, accidental causes of degeneracies of the minimum in the \( \Psi_0 \) space, but it is clear that the broken symmetry degeneracy has been removed by the projector \( P_0 \).

It is thus reasonable to assume that, provided all those symmetries broken by HF and similar approximations have been restored, a search for a minimum energy, \textit{after} the restoration, will suffer from no degeneracy any more.

Under this assumption of uniqueness of the minimum, consider the space of those \( \Psi_0 \) that are square normalized to unity. (This technicality spares us denominators.) Let \( \Psi_{0m} \) and \( \Psi_{0m}' \) be those states which provide \( F_m \) and \( F_m' \)
FIG. 1: One-to-one correspondence $u \leftrightarrow \rho$. A given potential $u$ (right) induces degenerate Slater determinant variational solutions (center) resulting in the same density $\rho$ after angular momentum projection (left).

for $H$ and $H'$ driven by distinct $u$ and $u'$, respectively. Then, the same argument *ab absurdo* as that for \[1\], with the same precaution of a non trivial difference between $u$ and $u'$,

\[
\int dr \left[ u(r) - u'(r) \right] \rho(r) = \langle \Psi_{0m} | (H - H') | \Psi_{0m} \rangle < F_m - F'_m,
\]

proves that $\Psi_{0m}$ and $\Psi'_{0m}$ cannot induce the same $\rho$. Hence the one-to-one map, $u \leftrightarrow \rho$, holds for the restricted variation space. It must be stressed here that the density $\rho$ is that of the symmetry projected state. It can differ from the density of every parent state $\phi$ through the correlations brought by the coherent summation over angles, Eq. (7).

The “smoothness” condition of $F$ around its minimum is necessary to allow for functional derivatives $\delta F_m/\delta u$, $\delta^2 F_m/(\delta u \delta u')$, etc. Since there are are no singularities in a space of Slater determinants (although this space is curved), and since that subset of determinants which might create singularities because of a vanishing matrix element $\langle \phi | P_0 | \phi \rangle$ has obviously a zero measure, we recover all the properties of the unrestricted variational space. In particular, $\delta F_m/\delta u = \rho$. A Legendre transform is possible. Hence there exists a functional of a spherical $\rho$, with value

\[
F_m = \langle \Psi_{0m} | (T + V) | \Psi_{0m} \rangle.
\]

It may be stressed here how a spherically invariant $u$ is in a one-to-one correspondence with a spherically invariant $\rho$. This is reassuring for the consistency of this existence theorem, deduced from a restricted variational space.

Since $\Psi_{0m}$ can only be an approximate ground state, then $F_m > F_M$, compare Eq. (3) without $\mu$ at $T = 0$ and Eq. (11). We are thus dealing with a new functional. It can only give upper bounds to bound state energies, but this is expected for restricted variational spaces, obviously.

For the case of nuclear forces, with their very repulsive core and need for short range correlations, nothing prevents us, formally at least, from refining the variational space by introducing a “correlator operator” *a la* Jastrow for instance, that crushes the wave function at short relative distances between particles,

\[
F_m = \min_{\phi} \frac{\langle \phi | C H C P_0 | \phi \rangle}{\langle \phi | C^2 P_0 | \phi \rangle}, \quad C = \prod_{i>j=1}^A \chi (|r_i - r_j|),
\]

\[1\]

\[2\]
where \( \chi \) vanishes at the origin and becomes 1 at large distances. Since \( C \) is a scalar, it commutes with \( P_0 \).

Our considerations can be easily generalized to finite temperatures, and to other symmetry restorations than angular momentum projections, and to other restricted spaces. It can be concluded that every restricted space and every symmetry restoration creates its own density functional, provided the conditions of uniqueness and smoothness of the variational minimum are fulfilled. For the discussion of differentiability and fine topological properties of the \( u \)- and \( \rho \) spaces we refer again to [8]. Up to our understanding, the validity of our existence theorems for symmetry conserving functionals is not compromised.

Such existence theorems, though, suffer from the usual plague of the field: constructive algorithms are missing.

Another question must now be raised: can one define a KS theory compatible with symmetry restoration? Consider again the case of angular momentum 0, for non degenerate ground states of scalar Hamiltonians, with \( \rho \) scalar, as are \( t, v \) and \( u \). One may then claim the exact \( F_M \) and its partner \( F_M \) are also scalar. Accordingly, all the tools of the KS theory, including the “under-rug-sweeping” exchange-correlation potential \( v_{xc}(r) \), must be rotationally invariant. For the sake of simplicity, let us forget spin-orbit complications. Then the KS equations read in coordinate space only,

\[
\left[ t + \int dr' v(r - r') \rho(r') + v_{xc}(r) + u(r) - \varepsilon_f \right] \varphi_{\ell m}(r) = 0,
\]

(13)

Can they be assumed to generate the same density as that of the correlated ground state?

In Eqs. (13), the magnetic degeneracy of the orbital eigenvalues \( \varepsilon_f \) is explicit. A complete filling of a core, made of all lowest shells but one, and a homogeneous, partial filling of a cloud for the residual particle number \( z \) in the next, partly filled shell, seem to be in order. It is trivial indeed that the following density,

\[
\rho(r) = \sum_{i \in \text{core}} |\varphi_i(r)|^2 + \frac{z}{2L + 1} \sum_{\ell \in \text{cloud}} |\varphi_{LM}(r)|^2,
\]

(14)

is rotationally invariant. Here \( L \) is the orbital label for the cloud, that first shell above the filled core, and \( M \) labels the corresponding degenerate orbitals. Can such a density be related to the angular momentum projection of any state in the subspace spanned by all the degenerate Slater determinants available when filling \( z \) among the degenerate \( 2L + 1 \) orbitals? Notice, incidentally, that necessarily \( z \neq 1 \) and \( z \neq 2L \), since such situations would only allow total angular momentum \( L \). Notice also that particle-hole symmetry that relates the coupling of angular momenta in a situation with \( 2L + 1 - z \) to that with \( z \). For simplicity, we thus set \( 2 \leq z \leq L \). Then we forget about the core and investigate the densities of those angular momentum projected determinants made of mixed orbitals inside the cloud. By mixed orbitals, we mean arbitrary linear superpositions of the magnetic numbers \( M \); such mixtures play the rôle of deformations. What is the density of such projected “deformed” determinants?

Consider \( L = 6, z = 4 \) for an illustrative example. Standard angular momentum techniques prove that one can then make two distinct states, \( \Psi_{0a} \) and \( \Psi_{0b} \), with total angular momentum 0. Therefore the projected Slater determinants must be linear combinations \( \alpha \Psi_{0a} + \beta \Psi_{0b} \), with densities \( \alpha^2 \rho_a + \beta^2 \rho_b + 2 \alpha \beta \rho_{ab} \), where \( \rho_{ab} \) is the “transition density”,

\[
\rho_{ab}(r) = \langle \Psi_{0b} | a_\downarrow r_\uparrow | \Psi_{0a} \rangle,
\]

(15)

while \( \rho_a \) and \( \rho_b \) are the densities of \( \Psi_a \) and \( \Psi_b \), respectively. The latter densities are the same, however. Indeed, since all orbitals have the same radial shape, \( \varphi(\rho) \), there are only angular integrals to consider when calculating the densities. For instance,

\[
\rho_a(r) = 4 \varphi(\rho)^2 \int d\hat{r}_2 d\hat{r}_3 d\hat{r}_4 |\psi_a(\hat{r}, \hat{r}_2, \hat{r}_3, \hat{r}_4)|^2,
\]

(16)

where \( \hat{r}_i \) designates the polar angles of a particle, and \( \psi_a \) carries the angular properties of \( \Psi_{0a} \). Because of the scalar nature of \( \rho_a \), it is obvious that the angular integral gives a result, \( \rho_a(r) = 4 \varphi(\rho)^2 \), which does not depend on the singled out \( \hat{r} \). The same holds for \( \Psi_{0b} \). Moreover, the transition density reads,

\[
\rho_{ab}(r) = 4 \varphi(\rho)^2 \int d\hat{r}_2 d\hat{r}_3 d\hat{r}_4 \psi_b(\hat{r}, \hat{r}_2, \hat{r}_3, \hat{r}_4)^* \psi_a(\hat{r}, \hat{r}_2, \hat{r}_3, \hat{r}_4),
\]

(17)

and this must again reduce to a constant with respect to \( \hat{r} \) because of the rotation invariance of both \( \Psi_{0a} \) and \( \Psi_{0b} \). The constant, however, must vanish. This is because, upon an integration with respect to \( r \), one must recover the
orthogonality of $\Psi_0$ and $\Psi_0$. It can be concluded that every “deformed” determinant made of orbitals taken from the spherical “cloud” shell has the same density. In Eq. (14), the sometimes called “filling” approximation term,

$$\frac{z}{2L+1} \sum_{M \in \text{cloud}} |\varphi_{LM}(r)|^2 = z \varphi(|r|)^2,$$

(18)

is not an approximation; it actually makes the exact ansatz for an exact, projected density.

The burden of an accurate description of $\rho$ then falls upon the radial shape $\varphi(|r|)$, that is the output of the KS equations, Eqs. (13). This makes it all the more important to better describe the often badly known potential $v_{xc}$.

Generalizations to other values of $L$ and $z$ and to more than two independent states with total angular momentum zero are obvious. All determinants from the cloud shell give the same density after projection.

To conclude, a word is in order about non spherical potentials $u$, and more generally symmetry breaking potentials $u$. As long as one is interested in Eq. (9), or rather in that proper form that takes into account the fact that $u$ does not commute any more with the symmetry restoring projector $P$, (still normalized to be idempotent,)

$$F_m = \text{Min}_\phi \frac{\langle \phi | \mathbf{P} \mathbf{H} \mathbf{P} | \phi \rangle}{\langle \phi | \mathbf{P} | \phi \rangle},$$

(19)

it is clear that only that symmetric part, $\mathbf{P}\mathbf{U}\mathbf{P}$, is activated. Hence a non symmetric $u$ brings nothing. The situation is different for the KS theory. Indeed, both the Hartree-like field, $\int dr' v(r-r') \rho(r')$, and a symmetry violating $u$ lift, in general, the unlikely degeneracies of the KS orbitals, and an unprojected density results from,

$$\left[ t + \int dr' v(r-r') \rho(r') + v_{xc}(r) + u(r) - \varepsilon_i \right] \varphi_i(r) = 0, \quad \rho(r) = \sum_i |\varphi_i(r)|^2.$$  

(20)

The sum, $\sum_i$, is taken, naturally, upon the lowest orbitals, except in very few anomalous cases. Consider a limit where $u$ becomes symmetric. As is well known, there is no reason why, at that limit, a symmetric state should emerge out of Eqs. (20). One needs an ansatz like Eq. (14) to enforce the symmetry. Under such an ansatz, which should be tuned for the partial filling of quasi degenerate orbitals, as with a finite temperature, the Hartree potential and a slightly symmetry violating $u$ will indeed create a slight degeneracy lifting only. There is thus a serious difference between an unconstrained KS approach and the symmetry constrained one.

To summarize this note, two distinct results are claimed, namely i) existence theorems for density functionals explicitly enforcing a symmetry by means of projectors chiseling variational spaces, and ii) a symmetry respectful version of the KS theory. The latter comes from an adjustment of the definition of the density; KS orbitals need to be incoherently mixed to account for symmetry projection.

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[1] T.L. Gilbert, Phys. Rev. B 12 (1975) 2111
[2] T. Duguet, private communication.
[3] P. Hohenberg and W. Kohn, Phys. Rev. 136 3B (1964) B864
[4] W. Kohn and L. J. Sham, Phys. Rev. 140 4A (1965) A1133
[5] N. D. Mermin, Phys. Rev. 137 A5 (1965) A1441
[6] R. van Leeuwen, Advances Quant. Chem. 43 (2003) 25; E.H. Lieb, Int. J. Quant. Chem. 24 (1983) 243; H. Englisch and R. Englisch, Phys. Stat. Solidi B123 (1984) 711 and B124 (1984) 373.
[7] B.G. Giraud, Constrained Orthogonal Polynomials, to be published by Journal of Physics A; B.G. Giraud, A. Weiguny and L. Wilets, Coordinates, Modes and Maps for the Density Functional, to be published by Nuclear Physics A.