The aim of density functional (DF) theory is to construct a functional that provides the energy expectation value for a correlated many-body state as a function of the one-body density. Thus, that minimization of the DF leads to the exact ground state (GS) density. Since the existence theorem proven for GSs by Hohenberg and Kohn (HK) [1], its extension by Mermin [2] to equilibrium at finite temperatures, and the further development by Kohn and Sham (KS) [3] of an equivalent, effective, independent particle problem, a considerable amount of work has been dedicated to generalizations such as spin DFs [4], functionals taking into account the symmetries of the Hamiltonian [5], calculations of excited state densities [6, 7], treatments of degeneracies or symmetries of the Hamiltonian [5], or an excited one, defines a density functional. Degeneracies created by a symmetry group can be trivially lifted by a pseudo-Zeeman effect. When complex scaling can be used to regularize a resonance into a square integrable state, a DF also exists.

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We show how every bound state of a finite system of identical fermions, whether a ground state or an excited one, determines a density functional. Degeneracies created by a symmetry group can be lifted by a pseudo-Zeeman effect. When complex scaling can be used to regularize a resonance into a square integrable state, a DF also exists.

### Existence of Density Functionals for Excited States and Resonances

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Existence of Density Functionals for Excited States and Resonances

The aim of density functional (DF) theory is to construct a functional that provides the energy expectation value for a correlated many-body state as a function of the one-body density, such that minimization of the DF leads to the exact ground state (GS) density. Since the existence theorem proven for GSs by Hohenberg and Kohn (HK) [1], its extension by Mermin [2] to equilibrium at finite temperatures, and the further development by Kohn and Sham (KS) [3] of an equivalent, effective, independent particle problem, a considerable amount of work has been dedicated to generalizations such as spin DFs [4], functionals taking into account the symmetries of the Hamiltonian [5], calculations of excited state densities [6, 7], treatments of degeneracies or symmetries of the Hamiltonian [5], or an excited one, defines a density functional. Degeneracies created by a symmetry group can be trivially lifted by a pseudo-Zeeman effect. When complex scaling can be used to regularize a resonance into a square integrable state, a DF also exists.
Consider now any excited bound eigenstate \( \psi_n \) of \( \mathbf{H} \), with its eigenvalue \( E_n \). Then, trivially, \( \psi_n \) is a GS of the semipositive definite operator \((\mathbf{H} - E_n)^2\). Since \( E_n \) is not known \emph{a priori}, consider rather an approximate value \( \tilde{E}_n \), obtained by any usual technique (configuration mixing, generator coordinates, etc.) and assume that \( \tilde{E}_n \) is closer to \( E_n \) than to any other eigenvalue \( E_p \). Then \( \psi_n \) is a GS of \((\mathbf{H} - \tilde{E}_n)^2\). The possible degeneracy degree of this GS is the same whether one considers \( \mathbf{H} \) or \((\mathbf{H} - \tilde{E}_n)^2\). Introduce now \( \mathbf{K} = (\mathbf{H} - \tilde{E}_n)^2 + \mathbf{W} \). If there is no degeneracy of either \( \psi_n \) or its continuation as a functional of \( w \), then the HK argument holds as well for \( \mathbf{K} \) as it does for \( \mathbf{H} \). Hence a trivial existence proof for a DF concerning \( \psi_n \). But most often, \( \psi_n \) belongs to a degenerate multiplet. Degeneracies are almost always due to an explicitly known symmetry group of \( \mathbf{H} \). Notice however that the external potential \( w \) does not need to show the same symmetry; hence, in general, for that subset of zero measure in the space of potentials where \( \psi_n \) emerges to minimize the expectation value of the symmetry group, or a chain of operators, precautions are necessary. Consider therefore an (or several) additional label(s) \( g \) sorting out the members \( \psi_{ng} \) of the multiplet corresponding to that eigenvalue \((E_n - \tilde{E}_n)^2\) of \((\mathbf{H} - \tilde{E}_n)^2\). There is always an operator \( \mathbf{G} \) related to the symmetry group, or a chain of operators \( \mathbf{G}_j \) in the reduction of the group by a chain of subgroups, which \emph{commute with} \( \mathbf{H} \) and can be chosen to define \( g \). For simplicity, assume that one needs to consider one \( \mathbf{G} \) only. Then define \( g \) as an eigenvalue of \( \mathbf{G} \) and assume, obviously, that the spectrum of \( \mathbf{G} \) is not degenerate, to avoid a reduction chain of subgroups. It is obvious that, given some positive constant \( C \), and given any chosen \( \gamma \) among the values of \( g \), there is no degeneracy for the GS of \((\mathbf{H} - \tilde{E}_n)^2 + C (\mathbf{G} - \gamma)^2 \). Nor is there a degeneracy of the GS of \( \mathbf{K} = (\mathbf{H} - \tilde{E}_n)^2 + C (\mathbf{G} - \gamma)^2 + \mathbf{W} = \mathbf{K} + C (\mathbf{G} - \gamma)^2 \), even if \( w \) has the symmetry. When several labels become necessary with a subgroup chain reduction, it is trivial to use a sum \( \sum_j C_j (\mathbf{G}_j - \gamma_j)^2 \) of “pusher” terms. Finally a DF results, now from the HK argument with \( \mathbf{K} \). We stress here that pusher terms, because they commute with \( \mathbf{H} \), do not change the \emph{eigenstates} of either \( \mathbf{H} \) nor \((\mathbf{H} - \tilde{E}_n)^2\). Only their \emph{eigenvalues} are sorted out and reorganized. Note that the pusher expectation value vanishes for \( \psi_{ng} \). Naturally, when \( w \) is finite, eigenstates of \( \mathbf{K} \) differ from those of \( \mathbf{H} \), but what counts is the information given by the DF when \( w \) vanishes. A simplification, avoiding cumbersome square operators \( \mathbf{H}^2 \), is worth noticing. Consider the operator, \( \mathbf{K} = \mathbf{H} + C (\mathbf{G} - \gamma)^2 + \mathbf{W} \). At the limit where \( w \) vanishes, there is always a choice of a positive constant \( C \) which makes the \emph{lowest} state with quantum number \( \gamma \) become the GS. This leads to a more restricted density functional that is of interest for the study of an yrast line.

That DF, \( F_M[\rho] \), based upon \( \mathbf{K} \), provides the expectation value, \( F_M[\rho] = \langle \psi_{min} | \left( (\mathbf{H} - \tilde{E}_n)^2 + C (\mathbf{G} - \gamma)^2 \right) | \psi_{min} \rangle \), where \( \psi_{min} \), square normalized to unity, is also constrained by the facts that \( \langle \psi_{min} | a_{\gamma}^\dagger a_{\gamma} | \psi_{min} \rangle = \rho(\gamma) \) and \( \mathbf{K} | \psi_{min} \rangle = \varepsilon | \psi_{min} \rangle \) for the eigenvalue \( \varepsilon = F_M \). It may be interesting to find a DF that provides the expectation value of \( \mathbf{H} \) itself. This can be done by taking the derivative of \( F_M[\rho] \) with respect to \( \tilde{E}_n \), at constant \( \rho \). We suppose that this derivative exists, which is the case for a discrete spectrum at least. With the notation \( | \psi \rangle = d|\psi\rangle/d\tilde{E}_n \), and using the fact that \( \langle \psi_{min} | \mathbf{W} | \psi_{min} \rangle + \langle \psi_{min} | \mathbf{W} | \psi_{min} \rangle = \int w(\tilde{r}) \left( d\rho(\tilde{r})/d\tilde{E}_n \right) d\tilde{r} = 0 \), one can write:

\[
\frac{dF_D[\rho]}{d\tilde{E}_n} = -\frac{2}{2} \langle \psi_{min} | (\tilde{E}_n - \mathbf{H}) | \psi_{min} \rangle + \\
\langle \psi_{min} | (\varepsilon - \mathbf{W}) | \psi_{min} \rangle + \langle \psi_{min} | (\varepsilon - \mathbf{W}) | \psi_{min} \rangle
\]

\[
= 2 \langle \psi_{min} | (\tilde{E}_n - \mathbf{H}) | \psi_{min} \rangle .
\]

Therefore we can define a new DF,

\[
F_D[\rho] = \tilde{E}_n - \frac{dF_M[\rho]}{2} d\tilde{E}_n,
\]

such that \( F_D[\rho] = \langle \psi_{min} | \mathbf{H} | \psi_{min} \rangle \) and \( F_D[\rho_{n\gamma}] = E_n \) for the density \( \rho_{n\gamma} \) of the eigenstate \( \psi_{n\gamma} \) of \( \mathbf{H} \) at energy \( E_n \). Furthermore one finds that \( \frac{\delta F_D[\rho]}{\delta \rho} (\rho_{n\gamma}) = 0 \), because \( \frac{\delta \langle \psi_{min} | \mathbf{H} | \psi_{min} \rangle}{\delta \rho} = E_n \frac{\delta \langle \psi_{min} | \psi_{min} \rangle}{\delta \rho} = 0 \) for \( \psi_{min} = \psi_{n\gamma} \). Hence the functional \( F_D[\rho] \) is stationary at the exact density \( \rho = \rho_{n\gamma} \). It is not expected to be minimal at \( \rho_{n\gamma} \), however, unless the resulting eigenstate corresponds to the absolute GS when \( w \) vanishes.

Resonances may be defined as special eigenstates of \( \mathbf{H} \) if one uses an argument à la Gamow, allowing some radial Jacobi coordinate \( r \geq 0 \) to show a diverging, exponential increase of the resonance wave function at infinity of the form \( \exp(ipr) \), where the channel momentum \( p \) is complex and \( \Im p < 0 \). It is well known that those eigenvalues \( E_n \) describing resonances are complex numbers, with \( \Im E_n < 0 \). There have been extensive discussions in the literature about the physical, or lack of, meaning of such non normalizable wave functions and about the wave packets which might be used to replace them. The point of view we adopt in this note is based upon the Complex Scaling Method (CSM) \[21, 22, 23, 24\]: a modest modification of \( \mathbf{H} \) transforms narrow resonances into \emph{square integrable} states; then there is no difference between the diagonalization for bound states and that for resonances. The cost of the CSM, however, is a loss of hermiticity: the CSM Hamiltonian \( \mathbf{H}' \) is non hermitian, somewhat similar to an optical Hamiltonian \[22, 23, 24\].

Given the ket eigenstate equation, \( (\mathbf{H} - E_n) | \psi_n \rangle = 0 \), where \( | \psi_n \rangle \) is now a square integrable resonance wave
function, we can consider the hermitian conjugate equation, \( \langle \psi_n | (H^\dagger - E_n^*) = 0 \). Clearly, \( \psi_n \) is a GS, as both a ket and a bra, of the hermitian and semipositive definite operator, \( Q_{\text{exact}} = (H^\dagger - E_n^*) (H^\dagger - E_n) \), with eigenvalue zero. Applying the same argument as before, but now to \( Q_{\text{exact}} \) instead of \( (H - E_n)^2 \), demonstrates the existence of a DF around the targeted resonant state.

In practice we do not know \( E_n \) exactly. Given a sufficiently close estimate \( E_n \) of \( E_n \), an approximate GS eigenvalue \( |E_n - \tilde{E}_n|^2 \) occurs for \( Q_{\text{apprx}} = (H^\dagger - \tilde{E}_n^*) (H^\dagger - \tilde{E}_n) \), at first order with respect to \( \Delta Q = Q_{\text{apprx}} - Q_{\text{exact}} \). Since \( \psi_n \) is not a ket eigenstate of \( H^\dagger = H^\dagger + i2i3H^\dagger, \) it is also perturbed at first order in \( \Delta Q \). Still one can copy the construction for \( \mathcal{F}_{D}[\rho] \), see Section 3, if one interprets the operators \( d/d\tilde{E}_n \) as \( d/d\tilde{E}_n + id/d3\tilde{E}_n \). The resulting functional \( \mathcal{F}_{D}[\rho] \) is linear in \( H^\dagger \). For \( E_n = E_n \) the functional will be stationary at the density of the exact resonant state. While providing a proof of existence, the construction of the exact functional for \( H^\dagger \) requires the knowledge of the exact eigenvalue \( E_n \). This might be an inconvenient limitation but fortunately calculations of numbers such as \( E_n \) are usually easier and much more precise than calculations of wave functions \( \psi_n \) and/or their densities.

If the resonance has good quantum numbers (QN)s inducing degeneracies, the same pusher terms as those which have been discussed above can be added to create a unique GS, from the operator, \( Q_{\text{exact}} + C (G - \gamma)^2 \). The HK argument, implemented with the full operator, \( K = (H^\dagger - E_n^*) (H^\dagger - E_n) + C (G - \gamma)^2 + W \), then proves that DFs exist for those resonances regularized by the CSM. Notice, however, that a simplified theory, with \( H^\dagger \) rather than \( H^\dagger + i2i3H^\dagger \), is here an integer and furthermore \( \rho_{LM} \) and \( \rho_{LM} \) are equal, and since Clebsch-Gordan coefficients have the symmetry property \( (LM L'M' | \lambda M'') = (-)^{LM} (L'M' L'M | \lambda M'') \), then necessarily \( \gamma = 0 \) if \( \lambda \) is odd. There are thus \( (L+1) \) scalar functions, \( \tau_0, \tau_2, \ldots, \tau_{2L} \), to parametrize \( (L+1) \) distinct densities \( \rho_{00}, \rho_{11}, \ldots, \rho_{LL} \). Because of the quadratic nature of the density observable, the even label \( \lambda \) for angular “modulation” of \( \rho \) runs from zero to \( \text{twice} L \), with a “2L cut-off”; a signature, necessary if not sufficient, for an “L-density”. Reinstate now \( \tilde{w} \) as the LT conjugate of \( \rho_{LM} \). It makes sense to study situations where \( \tilde{w} \) is restricted to expansions with \( (L+1) \) arbitrary scalar density factors, \( \tilde{w}(\tilde{r}) = \sum_{\gamma=0}^{2L-1} w_{\gamma}(\tilde{r}) \). With isoscalar factors such as \( (-)^{LM} (L - M L M | \lambda 0) \) omitted for simplicity in the following, every pair \( \{ \tau, \tilde{w} \} \) is conjugate. An eigenvalue \( \lambda \) of \( K \) or \( \tilde{K} \) may have an infinite number of multipole form factors, but, with such restricted potentials \( \rho_0 \), only \( \tau_0, \tau_2, \ldots, \tau_{2L} \) are chosen by the LT relating \( \mathcal{F}_{M} \) and \( F_{LM} \).

It can make even more sense to restrict \( \tilde{w} \) to one multipole only, \( \tilde{w}(\tilde{r}) = \tilde{w}_{\lambda}(\tilde{r}) \), with \( \lambda = 0, 2, \ldots, 2L \), to study each multipole of \( \rho \) separately. For simplicity we now use the easier version of the theory, with that operator \( K \) which is suited to the yrast line. Add therefore to \( H \) a pusher term \( Z_{LM} \) leaving intact the eigenstates, namely \( Z_{LM} = B [L L L + (L+1)]^2 + C (L - M)^2 \). Hence \( \tilde{K}_{LM} = \frac{K}{L+1} + \frac{W_{\lambda}}{V_{\lambda}} + \tilde{w}_{\lambda} + \frac{B}{V_{\lambda}} + \frac{W_{\lambda}}{V_{\lambda}} + C \). Here the subscript \( \lambda \) specifies that \( \tilde{w} \) is reduced to one multipole only. Then \( \tilde{L} \) is the total angular momentum operator and \( \tilde{L}_{z} \) is its third component. This operator \( Z_{LM} \) moves the eigenvalues of \( H \) so that the lowest eigenstate of \( H \) with quantum numbers \( \{LM \} \) becomes the GS of \( H + Z_{LM} \). The commutator \( [H, Z_{LM}] \) vanishes indeed, and given \( A, t, v \) and \( u \), there are always positive, large enough values for \( B \) and \( C \) that reshuﬄe the spectrum such that the lowest \( \{LM \} \) eigenstate \( \Psi_{LM} \) becomes the GS of \( H + Z_{LM} \) under this Zeeman-like effect. We stress again that \( Z_{LM} \) changes nothing in the eigenfunctions, eigendensities, etc., of all our Hamiltonians if \( w \) is rotationally invariant. Furthermore, angular momentum numbers remain approximately valid for eigenstates of \( \tilde{K}_{LM} \) if \( w \) is weak, and the same numbers might still make sense as labels by continuity when stronger deformations occur. Then the usual \textit{ad absurdum} argument
generates a map \( w_\lambda \leftrightarrow \tau_\lambda \), where \( \tau_\lambda (r) \) is the form factor of the \( \lambda \)-multipole component of the GS density for \( K_{L,M,\lambda} \), leading to an exact DF, for every \( \{LM\} \) lowest state and every even \( \lambda \) between \( 0 \) and \( 2L \). A generalization to operators \( K_{L,M,\lambda} \), involving \( (H - E_\lambda)^2 \), is trivial.

This note offers theorems for the existence of exact DFs for every excited bound state, and even narrow resonances, and every set of good QNs used in nuclear, atomic and molecular physics. Furthermore, the densities used as arguments of our DFs do not need to be fully two-body DFs, coming from the \( \delta \)-ally dedicated to calculations of the functional derivative, \( \delta \psi / \delta \rho (\vec{r}) \). Published studies of the KS formalism are actually dedicated to calculations of the functional derivative, \( \delta V_{xc} / \delta \rho (\vec{r}) \), of the exchange and correlation part of the DF, coming from the two-body part \( V \) of the DF. Our present use of modified Hamiltonians, or even squares of \( H \), introduces two-body operators, but also three- and four-body operators. For the versions where no squares of \( H \) occur, see the yrast suited operator \( K \) and Section 3, the nature of the three- and four-body terms, typically coming from \( (\vec{L} \vec{L})^2 \), is not forbidding, because of obvious factorization properties. Hence a KS theory might be realizable for such simplified versions. With squared Hamiltonians, however, a KS theory seems out of reach at present. A systematic analysis of solvable models on a basis of “modes” \(^{19}\), however, may help to extrapolate such models into practical rules. For the discussion of differentiability, representability and fine topological properties of the \( w \)- and \( p \)-spaces, we refer again to \(^{18}\).

Up to our understanding of the topology of the variational spaces, flat or curved \(^{29}\), of general use in nuclear, atomic and molecular theory, the validity domain of our existence theorems is quite large. We have not used the time dependent formalism, although much progress has been made in deriving excitation energies from it \(^{30}\). A generalization of our arguments to finite temperatures seems plausible, however, and insofar as inverse temperature may be viewed as an imaginary time, a generalization to a time dependent theory is not excluded.

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