Available online at www.sciencedirect.com
ScienceDirect
Physics Letters B 652 (2007) 69–72
PHYSICS LETTERS B
www.elsevier.com/locate/physletb

Existence of density functionals for excited states and resonances

B.G. Giraud [a,*], K. Katō [b], A. Ohnishi [b], S.M.A. Rombouts [c]

[a] *Service de Physique Théorique, DSM, CE Saclay, F-91191 Gif-sur-Yvette, France*
[b] *Division of Physics, Graduate School of Science, Hokkaido University, Sapporo 060-0810, Japan*
[c] *Ghent University, UGENT Department of Subatomic and Radiation Physics, Proeftuinstraat 86, B-9000 Gent, Belgium*

Received 16 January 2007; accepted 25 June 2007

Available online 6 July 2007

Editor: W. Haxton

Abstract

We show how every bound state of a finite system of identical fermions, whether a ground state 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.

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 excited states [8,9] and quasiparticles [10]. For the reader interested in an even more complete reading about both basic questions and applications, we refer to [11–19].

DFs for resonant states have received much less attention. We want to study this problem here. First we will address two related issues, namely that of a unified theory for ground and excited states and that of a theory for non-degenerate and degenerate ones. Then a generalized existence theorem can be constructed by modifying the Hamiltonian in such a way that the spectrum is shuffled but the eigenstates are left unchanged, and by making a systematic use of the Legendre transform (LT) for a detailed analysis of the density.

A reminder of the HK argument is useful here. Consider a finite number A of identical fermions, with $a^\dagger_{\vec r}$ and $a_{\vec r}$ their creation and annihilation operators at position $\vec r$, and the physical Hamiltonian, $\mathbf{H} = \mathbf{T} + \mathbf{V} + \mathbf{U}$, where $\mathbf{T} = \sum_{i=1}^{A} t_i$, $\mathbf{V} = \sum_{i>j=1}^{A} v_{ij}$ and $\mathbf{U} = \sum_{i=1}^{A} u_i$ are the kinetic, two-body interaction and one-body potential energies, respectively. For simplicity, we consider such fermions as spinless and isospinless and work at zero temperature. Both v and u may be either local or non-local. Next, embed the system into an additional one-body, external field, $\mathbf{W} = \sum_{i=1}^{A} w_i$, to observe its (non-linear!) response. The Hamiltonian becomes $\mathbf{K} = \mathbf{H} + \mathbf{W}$. It is understood that w is local, $\langle \vec r|w|\vec r'\rangle = w(r)\,\delta(\vec r - \vec r')$, although a DF theory with non-local potentials exists [20]. The usual Rayleigh–Ritz variational principle, where $|\psi\rangle$ is just an A-particle, antisymmetric, square normalized, otherwise unrestricted wave function, applied to $F_M = \min_\psi F$, with $F = \langle\psi|\mathbf{K}|\psi\rangle$, generates $\psi_{\min}$, the exact GS of $\mathbf{K}$, with the exact eigenvalue F_M. The minimum is assumed to be non-degenerate, smooth, reached. Clearly, $\psi_{\min}$ and F_M are parametrized by w. An infinitesimal variation δw triggers an infinitesimal displacement $\delta\psi_{\min}$, with $\delta F_M = \langle\psi_{\min}|\delta\mathbf{W}|\psi_{\min}\rangle$. There is no first order contribution from $\delta\psi_{\min}$. Define the one-body density ma-

* Corresponding author.
E-mail addresses: bertrand.giraud@cea.fr (B.G. Giraud), kato@nucl.sci.hokudai.ac.jp (K. Katō), ohnishi@nucl.sci.hokudai.ac.jp (A. Ohnishi), stefan.rombouts@rug.ac.be (S.M.A. Rombouts).

0370-2693/$ – see front matter
doi:10.1016/j.physletb.2007.06.071

trix in coordinate representation, $n(\vec{r},\vec{r}\,')=\langle\psi_{\min}|a^\dagger_{\vec{r}}a_{\vec{r}\,'}|\psi_{\min}\rangle$. Its diagonal, $\rho(\vec{r})=n(\vec{r},\vec{r})$, is the usual density deduced from $|\psi_{\min}|^2$ by integrating out all particles but one. Since $\delta F_M=\int d\vec{r}\,\rho(\vec{r})\delta w(\vec{r})$, then $\delta F_M/\delta w(\vec{r})=\rho(\vec{r})$. Freeze t, v and u and consider F_M as a functional of w alone. The HK process then consists in a *Legendre transform* of F_M, based upon this essential result, $\delta F_M/\delta w=\rho$. This LT involves two steps: (i) subtract from F_M the functional product of w and $\delta F_M/\delta w$, i.e. the integral $\int d\vec{r}\,w(\vec{r})\rho(\vec{r})$, leaving $\mathcal{F}_M=\langle\psi_{\min}|\mathbf{H}|\psi_{\min}\rangle$; then (ii) set ρ, the "conjugate variable of w", as the primary variable rather than w; hence see $\mathcal{F}_M$ as a functional of ρ. Step (ii) is made possible by the one-to-one ($1\leftrightarrow 1$) map between w and ρ, under precautions such as the exclusion of trivial variations δw that modify w by a constant only, see for instance [16] and [19]. The $1\leftrightarrow 1$ map is proven by the usual argument *ad absurdum* [1]: if distinct potentials w and w' generated $\psi_{\min}$ and $\psi'_{\min}$ (distinct!) with the same ρ, then two contradictory, strict inequalities would occur, $\int d\vec{r}\,[w(\vec{r})-w'(\vec{r})]\rho(\vec{r})<F_M-F'_M$, and, $\int d\vec{r}\,[w(\vec{r})-w'(\vec{r})]\rho(\vec{r})>F_M-F'_M$. An inverse LT returns from $\mathcal{F}_M$ to F_M, because $\delta\mathcal{F}_M/\delta\rho=-w$. Finally, the GS eigenvalue E_0 of $\mathbf{H}$ obtains as $E_0=\min_\rho\mathcal{F}_M[\rho]$; the GS wave function ψ_0 of $\mathbf{H}$ is the wave function $\psi_{\min}$ when w vanishes; that density providing the minimum of $\mathcal{F}_M$ is the density of ψ_0.

Consider now any excited bound eigenstate ψ_n of $\mathbf{H}$, with its eigenvalue E_n. Then, trivially, ψ_n is a GS of the semipositive definite operator $(\mathbf{H}-E_n)^2$. Since E_n is not known *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 ψ_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 $\tilde{\mathbf{K}}=(\mathbf{H}-\tilde{E}_n)^2+\mathbf{W}$. If there is no degeneracy of either ψ_n or its continuation as a functional of w, then the HK argument holds as well for $\tilde{\mathbf{K}}$ as it does for $\mathbf{K}$. Hence a trivial existence proof for a DF concerning ψ_n. But most often, ψ_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 $\tilde{\mathbf{K}}$, there is no degeneracy of its GS; a unique $\psi_{\min}$ emerges to minimize the expectation value of $\tilde{\mathbf{K}}$. However, for that subset in the space of potentials where w shows the symmetry responsible for the degeneracy, and in particular for the limit $w\to 0$, precautions are necessary. Consider therefore an (or several) additional label(s) g sorting out the members ψ_{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 *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 γ 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 $\bar{\mathbf{K}}=(\mathbf{H}-\tilde{E}_n)^2+C(\mathbf{G}-\gamma)^2+\mathbf{W}=\tilde{\mathbf{K}}+C(\mathbf{G}-\gamma)^2$, 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. A DF results, now from the HK argument with $\bar{\mathbf{K}}$. We stress here that pusher terms, because they commute with $\mathbf{H}$, do not change the *eigenstates* of either $\mathbf{H}$ nor $(\mathbf{H}-\tilde{E}_n)^2$. Only their *eigenvalues* are sorted out and reorganized. Note that the pusher expectation value vanishes for $\psi_{n\gamma}$. Naturally, when w is finite, eigenstates of $\bar{\mathbf{K}}$ differ from those of $\tilde{\mathbf{K}}$, 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, $\hat{\mathbf{K}}=\mathbf{H}+C(\mathbf{G}-\gamma)^2+\mathbf{W}$. At that limit, $w\to 0$, there is always a choice of a positive constant C which makes the *lowest* state with quantum number γ become the GS. This leads to a more restricted density functional, of interest for the study of an yrast line.

That DF, $\mathcal{F}_M[\rho]$, based upon $\bar{\mathbf{K}}$, provides the expectation value, $\mathcal{F}_M[\rho]=\langle\psi_{\min}|[(\mathbf{H}-\tilde{E}_n)^2+C(\mathbf{G}-\gamma)^2]|\psi_{\min}\rangle$, where $\psi_{\min}$, square normalized to unity, is also constrained by the facts that $\langle\psi_{\min}|a^\dagger_{\vec{r}}a_{\vec{r}}|\psi_{\min}\rangle=\rho(\vec{r})$ and $\bar{\mathbf{K}}|\psi_{\min}\rangle=\varepsilon|\psi_{\min}\rangle$ 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 $\mathcal{F}_M[\rho]$ with respect to $\tilde{E}_n$, *at constant* ρ. We suppose that this derivative exists, which is the case for a discrete spectrum at least. With the notation $|\dot{\psi}\rangle=d|\psi\rangle/d\tilde{E}_n$, and using the fact that $\langle\psi_{\min}|\mathbf{W}|\dot{\psi}_{\min}\rangle+\langle\dot{\psi}_{\min}|\mathbf{W}|\psi_{\min}\rangle=\int w(\vec{r})(d\rho(\vec{r})/d\tilde{E}_n)\,d\vec{r}=0$, one can write:

$$\begin{aligned}\frac{d\mathcal{F}_M[\rho]}{d\tilde{E}_n}&=2\langle\psi_{\min}|(\tilde{E}_n-\mathbf{H})|\psi_{\min}\rangle\\&\quad+\langle\dot{\psi}_{\min}|(\varepsilon-\mathbf{W})|\psi_{\min}\rangle+\langle\psi_{\min}|(\varepsilon-\mathbf{W})|\dot{\psi}_{\min}\rangle\\&=2\langle\psi_{\min}|(\tilde{E}_n-\mathbf{H})|\psi_{\min}\rangle.\end{aligned}\tag{1}$$

Therefore we can define a new DF,

$$\mathcal{F}_D[\rho]=\tilde{E}_n-\frac{d\mathcal{F}_M[\rho]}{2d\tilde{E}_n},\tag{2}$$

such that $\mathcal{F}_D[\rho]=\langle\psi_{\min}|\mathbf{H}|\psi_{\min}\rangle$ and $\mathcal{F}_D[\rho_{n\gamma}]=E_n$ for the density $\rho_{n\gamma}$ of the eigenstate $\psi_{n\gamma}$ of $\mathbf{H}$ at energy E_n. Furthermore one finds that $\frac{\delta\mathcal{F}_D}{\delta\rho}[\rho_{n\gamma}]=0$, because $\frac{\delta\langle\psi_{\min}|}{\delta\rho}\mathbf{H}|\psi_{\min}\rangle+\langle\psi_{\min}|\mathbf{H}\frac{\delta|\psi_{\min}\rangle}{\delta\rho}=E_n\frac{\delta\langle\psi_{\min}|\psi_{\min}\rangle}{\delta\rho}=0$ for $\psi_{\min}=\psi_{n\gamma}$. Hence the functional $\mathcal{F}_D[\rho]$ 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 $r\geqslant 0$ 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, [21–24]. The point of view we adopt in this note is based upon the Complex Scaling Method (CSM) [25–28]: a modest modification of $\mathbf{H}$ transforms narrow resonances into *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; it is somewhat similar to an optical Hamiltonian [25–28].

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, $\langle\psi_n|(\mathbf{H}'^{\dagger} - E_n^*) = 0$. Clearly, ψ_n is a GS, as both a ket and a bra, of the Hermitian and semipositive definite operator, $\mathbf{Q}_{\text{exact}} = (\mathbf{H}'^{\dagger} - E_n^*)(\mathbf{H}' - E_n)$, with eigenvalue 0. Applying the same argument as before, but now to $\mathbf{Q}_{\text{exact}}$ instead of $(\mathbf{H}-\tilde{E}_n)^2$, demonstrates the existence of a DF around the targeted resonant state.

In practice one does not know E_n exactly. Given a sufficiently close estimate $\tilde{E}_n$ of E_n, an approximate GS eigenvalue $|E_n - \tilde{E}_n|^2$ occurs for $\mathbf{Q}_{\text{apprx}} = (\mathbf{H}'^{\dagger} - \tilde{E}_n^*)(\mathbf{H}' - \tilde{E}_n)$, at first order with respect to $\Delta\mathbf{Q} = \mathbf{Q}_{\text{apprx}} - \mathbf{Q}_{\text{exact}}$. Since ψ_n is not a ket eigenstate of $\mathbf{H}'^{\dagger} = \mathbf{H}' - 2i\Im\mathbf{H}'$, it is also perturbed at first order in $\Delta\mathbf{Q}$. Still one can copy the construction for $\mathcal{F}_D[\rho]$, see Eq. (2); one interprets the operator $\mathrm{d}/\mathrm{d}\tilde{E}_n^*$ as $\mathrm{d}/\mathrm{d}\Re\tilde{E}_n + i\,\mathrm{d}/\mathrm{d}\Im\tilde{E}_n$. The resulting functional $\mathcal{F}_D[\rho]$ is linear in $\mathbf{H}'$. For $\tilde{E}_n = E_n$ 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 $\mathbf{H}'$ 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 much easier and much more precise than calculations of wave functions ψ_n and/or of their densities.

If the resonance has good quantum numbers (QNs) inducing degeneracies, the same pusher terms as those which have been discussed above can be added to create a unique GS, from the operator, $\mathbf{Q}_{\text{exact}} + C(\mathbf{G}-\gamma)^2$. The HK argument, implemented with the full operator, $\bar{\mathbf{K}}' = (\mathbf{H}'^{\dagger} - E_n^*)(\mathbf{H}' - E_n) + C(\mathbf{G} - \gamma)^2 + \mathbf{W}$, then proves that DFs exist for those resonances regularized by the CSM. Notice, however, that a simplified theory, with an "yrast suited" operator $\hat{\mathbf{K}}'$, linear with respect to $\mathbf{H}'$, is not available here, since the restoration of Hermiticity forces a product $\mathbf{H}'^{\dagger}\mathbf{H}'$ upon our formalism.

Now consider a special case of rather wide interest in nuclear and atomic physics. (i) Good parity of eigenstates of $\mathbf{H}_0 = \mathbf{T} + \mathbf{V}$ or $\mathbf{H} = \mathbf{H}_0 + \mathbf{U}$ when u is restricted to be even, is assumed in the following. Hence now eigendensities, quadratic with respect to the states, have positive parities. (ii) Also assume that the number of fermions is even. (iii) The QNs in which we are interested in this section are the integer angular momentum L and magnetic label M of an eigenstate Ψ_{LM} of $\mathbf{H}$, where it is understood that the two-body v and one-body u interactions conserve angular momentum. When w is switched on and is not rotationally invariant, eigenstates of $\mathbf{K}$, $\tilde{\mathbf{K}}$, or $\bar{\mathbf{K}}$ may still tolerate such labels LM by continuity. First, consider $w = 0$. The density ρ_{LM} comes from the product $\Psi_{LM}^*\Psi_{LM}$, but it does not transform under rotations as an $\{LM\}$ tensor. Rather, it is convenient to define "auxiliary densities", $\sigma_{\lambda 0}(\vec{r}) = \sum_{M=-L}^{L} (-)^{L-M}\langle L - MLM|\lambda 0\rangle \rho_{LM}(\vec{r})$, where $\langle L - MLM|\lambda 0\rangle$ is a usual Clebsch–Gordan coefficient. Each function $\sigma_{\lambda 0}(\vec{r})$ now behaves under rotations as a $\{\lambda 0\}$ tensor. It can therefore be written as the product of a spherical harmonic and a radial form factor, $\sigma_{\lambda 0}(\vec{r}) = Y_{\lambda 0}(\hat{r})\tau_\lambda(r) = \sqrt{(2\lambda+1)/4\pi}\,\mathcal{L}_\lambda(\cos\beta)\tau_\lambda(r)$, where $\mathcal{L}_\lambda$ is a Legendre polynomial and the angle β is the usual polar angle, counted from the z-axis. Conversely,

$$\rho_{LM}(\vec{r}) = \sum_{\lambda=0}^{2L} (-)^{L-M}\langle L - MLM|\lambda 0\rangle Y_{\lambda 0}(\hat{r})\tau_\lambda(r). \tag{3}$$

This makes a "Fourier analysis" in angular space. *Scalar* form factors τ_λ parametrize ρ_{LM}. Since L is here an integer and furthermore $\rho_{L-M} = \rho_{LM}$, and since Clebsch–Gordan coefficients have the symmetry property $\langle LML'M'|\lambda M''\rangle = (-)^{L+L'-\lambda}\langle L'M'LM|\lambda M''\rangle$, then $\tau_\lambda = 0$ for λ odd. There are thus $(L+1)$ scalar functions, $\tau_0, \tau_2, \ldots, \tau_{2L}$, to parametrize $(L+1)$ distinct densities $\rho_{L0}, \rho_{L1}, \ldots, \rho_{LL}$. Because of the quadratic nature of the density, the even λ for angular "modulation" of ρ runs from 0 to *twice* L, with a "$2L$ cut-off"; a signature, necessary if not sufficient, for an "L-density". Reinstate now w as the LT conjugate of ρ_{LM}. It makes sense to restrict w to expansions with $(L+1)$ arbitrary scalar form factors, $w(\vec{r}) = \sum_{\text{even}\lambda=0}^{2L} Y_{\lambda 0}(\hat{r})w_\lambda(r)$. With inessential factors $(-)^{L-M}\langle L - MLM|\lambda 0\rangle$ omitted, every pair $\{r\tau_\lambda, rw_\lambda\}$ is conjugate. An eigendensity of $\mathbf{K}$, $\tilde{\mathbf{K}}$, $\bar{\mathbf{K}}$ may have an infinite number of multipole form factors, but, with such a restricted w, only $\tau_0, \tau_2, \ldots, \tau_{2L}$ are chosen by the LT relating $\mathcal{F}_M$ and F_M.

It can make even more sense to restrict w to one multipole only, $w(\vec{r}) = Y_{\lambda 0}(\hat{r})w_\lambda(r)$, with $\lambda = 0$, or $2, \ldots$ or $2L$, to study each multipole of ρ separately. For simplicity we now use the easier version of the theory, with that operator $\hat{\mathbf{K}}$ which is suited to the yrast line. Add therefore to $\mathbf{H}$ a pusher term $\mathbf{Z}_{LM}$ leaving intact the eigenstates, namely $\mathbf{Z}_{LM} = B[\vec{\mathbf{L}}\cdot\vec{\mathbf{L}} - L(L+1)]^2 + C(\mathbf{L}_z - M)^2$. Hence $\hat{\mathbf{K}}_{LM\lambda} = \mathbf{H} + \mathbf{Z}_{LM} + \mathbf{W}_\lambda = \mathbf{T} + \mathbf{V} + \mathbf{U} + \mathbf{Z}_{LM} + \mathbf{W}_\lambda$. Here the subscript λ specifies that w is reduced to one multipole only, then $\vec{\mathbf{L}}$ is the total angular momentum operator and $\mathbf{L}_z$ is its third component. This operator $\mathbf{Z}_{LM}$ moves the eigenvalues of $\mathbf{H}$ so that the lowest eigenstate of $\mathbf{H}$ with quantum numbers $\{LM\}$ becomes the GS of $\mathbf{H} + \mathbf{Z}_{LM}$. The commutator $[\mathbf{H}, \mathbf{Z}_{LM}]$ 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 Ψ_{LM} becomes the GS of $\mathbf{H} + \mathbf{Z}_{LM}$ under this Zeeman-like effect. We stress again that $\mathbf{Z}_{LM}$ 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 $\hat{\mathbf{K}}_{LM\lambda}$ if w is weak, and the same numbers might still make sense as labels by continuity when stronger deformations occur. Then the usual *ad absurdum* argument generates a map $w_\lambda \leftrightarrow \tau_\lambda$, where $\tau_\lambda(r)$ is the form factor of the λ-multipole component of the GS density for $\hat{\mathbf{K}}_{LM\lambda}$, leading to an *exact* DF, for every $\{LM\}$ lowest state and every even λ between 0 and $2L$. A generalization to operators $\bar{\mathbf{K}}_{LM\lambda}$, involving $(\mathbf{H} - \tilde{E}_n)^2$, is trivial.

This note thus offers theorems for the *existence* of exact DFs for every excited bound state, and even narrow resonances, and every set of good QNs. Furthermore, the densities used as arguments of our DFs do not need to be fully three-dimensional ones; they can be radial form factors of multipole components of the studied states.

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 is plausible, however, and insofar as inverse temperature may be viewed as an imaginary time, a time dependent theory is not excluded.

For the discussion of differentiability, representability and fine topological properties of the w- and ρ-spaces, we refer again to [16]. 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.

Such theorems, though, suffer from the usual plague of the field: constructive algorithms are missing. Empirical approaches are necessary. Is there a corresponding Kohn–Sham theory (KST) [3]? In the usual KST, the calculation of the kinetic energy part of the DF is left to the solution of Hartree-like equations. Besides the kinetic operator, the KS equations contain a Hartree potential, completed by a potential modeling exchange and correlation. Published KST formalisms are dedicated to estimates of the functional derivative, $\delta\mathcal{V}_{xc}/\delta\rho(\vec{r})$, of the exchange and correlation part of the DF, coming from the *two-body* part $\mathcal{V}$ of the DF. This can be generalized, formally at least. Our use of modified Hamiltonians, or even squares of $\mathbf{H}$, introduces one-, two-, three- and four-body operators, $\mathcal{O}_1$, $\mathcal{O}_2$, $\mathcal{O}_3$ and $\mathcal{O}_4$, respectively. It is trivial to build a KS Hamiltonian $\mathcal{H}$ by retaining $\mathcal{O}_1$ and those Hartree operators coming from local parts of $\mathcal{O}_2$, $\mathcal{O}_3$ and $\mathcal{O}_4$. Then one has to complete $\mathcal{H}$ by designing generalizations of $\delta\mathcal{V}_{xc}/\delta\rho(\vec{r})$ including terms from the non-Hartree parts relating to $\mathcal{O}_2$, $\mathcal{O}_3$ and $\mathcal{O}_4$. For our theorems where no squares of $\mathbf{H}$ occur, see the yrast suited operator $\hat{\mathbf{K}}$ and Eq. (2), the nature of $\mathcal{O}_2$, $\mathcal{O}_3$, and $\mathcal{O}_4$, typically coming from $(\vec{\mathbf{L}}\,.\,\vec{\mathbf{L}})^2$, is not forbidding, because of obvious factorization properties. Hence a KST might be realizable for such a simpler case. With squared Hamiltonians, however, a KST seems more remote at present and one must have to be content, temporarily at least, with just existence theorems. A systematic analysis of solvable models on a basis of "modes" [19], however, may help to extrapolate such models into practical rules.

Acknowledgements

B.G.G. thanks the hospitality of the Hokkaido University and Kyoto Yukawa Institute for part of this work. S.M.A.R. thanks D. Van Neck for interesting discussions.

References

[1] P. Hohenberg, W. Kohn, Phys. Rev. 136 (1964) B864.
[2] N.D. Mermin, Phys. Rev. 137 (1965) A1441.
[3] W. Kohn, L.J. Sham, Phys. Rev. 140 (1965) A1133.
[4] O. Gunnarson, B.J. Lundquist, Phys. Rev. B 13 (1976) 4274.
[5] A. Görling, Phys. Rev. A 47 (1993) 2783.
[6] A. Görling, Phys. Rev. A 59 (1999) 3359.
[7] M. Levy, Á. Nagy, Phys. Rev. Lett. 83 (1999) 4361.
[8] A. Görling, Phys. Rev. Lett. 85 (2000) 4229.
[9] Á. Nagy, M. Levy, Phys. Rev. A 63 (2001) 052502.
[10] D. Van Neck, et al., Phys. Rev. A 74 (2006) 042501.
[11] J. Dobaczewski, H. Flocard, J. Treiner, Nucl. Phys. A 422 (1984) 103.
[12] J. Meyer, J. Bartel, M. Brack, P. Quentin, S. Aicher, Phys. Lett. B 172 (1986) 122.
[13] R.M. Dreizler, E.K.U. Gross, Density Functional Theory, Springer, Berlin, 1990.
[14] Rambir Singh, D.M. Deb, Phys. Rep. 311 (1999) 47.
[15] J.P. Perdew, S. Kurth, in: C. Fiolhais, F. Nogueira, M. Marques (Eds.), A Primer in Density Functional Theory, in: Lecture Notes in Physics, vol. 620, Springer, Berlin, 2003, see also the references in their review.
[16] R. van Leeuwen, Adv. Quantum Chem. 43 (2003) 25;
E.H. Lieb, Int. J. Quantum Chem. 24 (1983) 243;
H. Englisch, R. Englisch, Phys. Status Solidi B 123 (1984) 711;
H. Englisch, R. Englisch, Phys. Status Solidi B 124 (1984) 373.
[17] T. Duguet, Phys. Rev. C 67 (2003) 044311;
T. Duguet, P. Bonche, Phys. Rev. C 67 (2003) 054308.
[18] G.F. Bertsch, B. Sabbey, M. Uusnäkki, Phys. Rev. C 71 (2005) 054311.
[19] B.G. Giraud, J. Phys. A 38 (2005) 7299;
B.G. Giraud, A. Weiguny, L. Wilets, Nucl. Phys. A 61 (2005) 22;
B.G. Giraud, M.L. Mehta, A. Weiguny, C. R. Phys. 5 (2004) 781.
[20] T.L. Gilbert, Phys. Rev. B 12 (1975) 2111.
[21] N.S. Krylov, V.A. Fock, Zh. Eksp. Teor. Fiz. 17 (1947) 93.
[22] L. Fonda, G.C. Ghirardi, A. Rimini, Rep. Prog. Phys. 41 (1978) 587.
[23] V.J. Menon, A.V. Lagu, Phys. Rev. Lett. 51 (1983) 1407.
[24] T. Berggren, Phys. Lett. B 373 (1996) 1.
[25] Y.K. Ho, Phys. Rep. 99 (1983) 1, see also the reference list of this review paper.
[26] N. Moiseyev, Phys. Rep. 302 (1998) 211, see also the reference list of this review paper.
[27] T. Myo, A. Ohnishi, K. Katō, Prog. Theor. Phys. 99 (1998) 801;
T. Myo, K. Katō, S. Aoyama, K. Ikeda, Phys. Rev. C 63 (2001) 054313.
[28] B.G. Giraud, K. Katō, Ann. Phys. 308 (2003) 115;
B.G. Giraud, K. Katō, A. Ohnishi, J. Phys. A 37 (2004) 11575.
[29] B.G. Giraud, D.J. Rowe, J. Phys. Lett. 40 (1979) L177;
B.G. Giraud, D.J. Rowe, Nucl. Phys. A 330 (1979) 352.
[30] M. Petersilka, U.J. Gossmann, E.K.U. Gross, Phys. Rev. Lett. 76 (1996) 1212.