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ORIGINAL PAPER

Variational principle, Hohenberg–Kohn theorem, and density function origin shifts

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Abstract Origin shifts performed on the density functions (DF) permit to express the Hohenberg–Kohn theorem (HKT) as a consequence of the variational principle. Upon ordering the expectation values of Hermitian operators, an extended variational principle can be described using origin shifted DF. Under some restrictions, HKT can be extended for some specific Hermitian operators.

Keywords Density function origin shift · Variational principle · Hohenberg–Kohn Theorem · Extended variational principle

1 Introduction

Since the publication of Hohenberg–Kohn theorem (HKT) [1] and its mathematical development by Lieb [2], the structure and properties of HKT has been studied by many researches in the field, including the original authors, see for example references [3–13]. Coincident with the turn of the century we published some work [14] on HKT and accompanied it by the discussion of an equivalent matrix theorem [15]. This work was followed by studies on the nature of the relation between wave and density functions in the framework of Schrödinger equation formalism [16–18].

Later on, our interest on HKT was aroused by previous work of Mezey on holographic electronic density theorem (HEDT) [19] and the link of the HEDT with HKT disclosed by the same author [20]. Such previous Mezey's work has been the inspiration of several papers [21–24] issued from our laboratory.

Recent experience [25–28] indicates that, when dealing with density function (DF) sets composed by two or more elements, one might geometrically rearrange the DF set

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members within the containing Hilbert semispace [29–31]. This can be done shifting them with respect to another chosen DF-like form, which can be selected taking any element within the DF set or chosen as being a composite of them, for instance, the centroid DF attached to the studied DF set or any other convex combination of the DF set elements.

The present work corresponds to the analysis of another application of the mentioned DF origin shift technique. For this purpose it will be also used the formalism developed several years ago concerning expectation values and DF [16,32–34]. Within such formal development, considering any arbitrary quantum system, it is used the fact that any Hermitian operator expectation value can be computed with the application of the operator on the appropriate DF, followed by integration over the existence domain. Such expectation value formalism has to be considered the basic mathematical structure complementing the origin shift in the present study.

Therefore, after some introduction to the DF origin shift technique, the aim of the present work first will be to describe how the variational principle can be extended to any Hermitian operator and second how Hohenberg–Kohn theorem (HKT) can be deduced from this mathematical formalism. It will be proved how HK theorem can be inferred from the variational principle, which in turn can be considered as a consequence of the involved operator expectation values ordering.

2 Origin shift of DF sets

2.1 DF sets and convex combinations

In fact, as it has been commented in the introduction, one can choose any function to be used as origin shift of a DF set, provided it bears the main features DF possess. So, composite functions obtained using any convex linear combination of DF [25–28] can be considered as good candidates for origin shift purposes.

A set of DF can be written as: $\mathbb{P} = \{\rho_I \,|I = 1, N\}$, where the set elements are non-negative functions with well-defined positive definite Minkowski norms[1]: $\forall I$: $\langle \rho_I \rangle = v_I \in \mathbf{R}^+$. A convex set of positive real numbers: $\mathbb{A} = \{\alpha_I \,|I = 1, N\} \subset [0, 1]$ has the essential additional property: $\sum_I \alpha_I = 1$, which it is the same to consider the coefficient set $\mathbb{A}$ as a discrete probability distribution.

Then, taking these definitions into account, a convex linear combination of DF can be written as:

$$\rho = \sum_I \alpha_I \rho_I \rightarrow \langle \rho \rangle = \sum_I \alpha_I \langle \rho_I \rangle = \sum_I \alpha_I v_I \in \mathbf{R}^+, \tag{1}$$

which proves that the Minkowski norm of the composite function can be taken as a mean value of the norms of the DF set elements. Note that if the DF set $\mathbb{P}$ corresponds

[1] Any integrable multivariate function $f(\mathbf{r})$ can be used with the symbol: $\langle f(\mathbf{r}) \rangle = \int_D f(\mathbf{r})\, d\mathbf{r}$, which will be employed along this paper. If the integral result is positive definite, then $\langle f \rangle$ corresponds to the Minkowski norm of the involved function, if not it can be called a Minkowski pseudo-norm.

to shape functions, for which: $\forall I : \langle \rho_I \rangle = 1$, then the convex linear combination (1) is also like a shape function as in this case will hold the norm: $\langle \rho \rangle = 1$.

2.2 Origin shifts in a minimal DF set

Origin shift of DF sets essentially uses DF differences [25–28]. Hence, in order to study a minimal origin shift scenario, at least a two DF set, say: $\mathbb{P} = \{\rho_0; \rho_a\}$, is needed to be taken into account as origin shift candidate, but providing a schematic but sufficiently adequate DF origin shift example.

Then, considering the case of a DF set constructed with only two elements, one can build the convex family of functions:

$$\forall \alpha \in [0, 1] : \rho_\alpha = \alpha \rho_a + (1 - \alpha)\, \rho_0 = \rho_0 + \alpha\, (\rho_a - \rho_0)\,,$$

or alternatively an equivalent convex family can be also constructed:

$$\forall \beta \in [0, 1] : \rho_\beta = \beta \rho_0 + (1 - \beta)\, \rho_a = \rho_a + \beta\, (\rho_0 - \rho_a)\,.$$

In both convex linear combination definitions the most relevant role is played by the difference of the two involved DF in the set:

$$\zeta_{a0} = \rho_a - \rho_0 = -\zeta_{0a} \leftrightarrow \zeta_{0a} = \rho_0 - \rho_a = -\zeta_{a0};$$

Such a result meaning that upon origin shift, the DF original pair becomes a *unique* shifted DF (SDF). This can be formally written as a transformation of the original DF set:

$$\Xi\,(\mathbb{P}) = \Xi\,\{\rho_0; \rho_a\} \rightarrow \{\zeta_{0a}\}\,.$$

The common property to any DF consists of being definite non-negative. However, any resulting SDF possess a non-definite character. Such situation designs the essential features of the origin shift process and the SDF main peculiarity with respect to any attached DF.

Now it is also interesting to note the effect of the previously defined convex linear combinations, when employed as origin shifts. Recalling the earlier SDF obtained in the minimal DF set made of two DF as elements:

$$\zeta = \zeta_{a0} \rightarrow -\zeta = \zeta_{0a},$$

then it can be also written:

$$\begin{aligned} \rho_0 - \rho_\alpha &= \alpha\, (\rho_0 - \rho_a) = -\alpha \zeta \\ \rho_0 - \rho_\beta &= (1 - \beta)\, (\rho_0 - \rho_a) = (\beta - 1)\, \zeta, \end{aligned}$$

and alternatively

$$\rho_a - \rho_\alpha = (1-\alpha)(\rho_a - \rho_0) = (1-\alpha)\zeta$$
$$\rho_a - \rho_\beta = \beta(\rho_a - \rho_0) = \beta\zeta.$$

The equalities shown above, demonstrate that in general, origin shifts yield, when performed upon any two DF set $\mathbb{P}$, a unique scalar multiple of the attached SDF: ζ.

2.3 Centroid shift

As a particular case of the previously discussed two DF convex combinations, the centroid DF can be constructed in the following way:

$$\rho_C = \frac{1}{2}(\rho_0 + \rho_a).$$

Then the origin shifts produced by this centroid DF can be written like a particular result of the general ones, as obtained in the previous discussion, that is:

$$\rho_0 - \rho_C = \rho_0 - \frac{1}{2}(\rho_0 + \rho_a) = \frac{1}{2}(\rho_0 - \rho_a) = -\frac{1}{2}\zeta$$
$$\rho_a - \rho_C = \rho_a - \frac{1}{2}(\rho_0 + \rho_a) = \frac{1}{2}(\rho_a - \rho_0) = \frac{1}{2}\zeta.$$

Besides the fact that non-negative definition of the DF elements is lost in SDF sets, this last result is also consistent with a universal property of DF sets (and in general of any kind of vector sets) [25], which states that upon any origin shift, the original linearly independent DF set is reduced in one dimension.

Thus, when considering sets of two DF, the origin shift transforms them into a SDF set of only one element, without a proper definite structure and lacking of strictly positive Minkowski norm, but a pseudo-norm. It is easy to see that: $\langle\zeta\rangle = \langle\rho_a - \rho_0\rangle = \langle\rho_a\rangle - \langle\rho_0\rangle = v_a - v_0 \in \mathbf{R}$.

2.4 Comparison of two DF

2.4.1 Euclidian distance

At the light of these preliminary findings, the comparison of two DF seems irrelevant. This dual comparison, as a result of the previous discussion, can be resumed by a unique SDF, which is the difference of the compared ones. Comparison of DF, attached to the same quantum object system (in molecular structures, for instance, this can be obtained by different procedures or AO basis set levels), in fact produces a SDF with a null Minkowski pseudo-norm.

However, the SDF selfsimilarity, which is coincident with the Euclidian norm, yields:

$$\begin{aligned}\langle|\zeta|^2\rangle &= \langle|\rho_a - \rho_0|^2\rangle = \langle|\rho_a|^2\rangle - 2\langle\rho_0\rho_a\rangle + \langle|\rho_0|^2\rangle \\ &= Z_{aa} - 2Z_{0a} + Z_{00} = D_{0a}^2.\end{aligned}$$

So it is found a final expression, which is coincident with the squared Euclidian distance between both DF, and at the same time measures the degree of dissimilarity between the two initial DF.

An interesting case within LCAO MO framework is constituted by two DF of the same quantum object electronic state, obtained under the same basis set, but using different computational methods. In this circumstance the SDF can be written as:

$$\zeta = \sum_{\mu}\sum_{\nu}\left(D_{0,\mu\nu} - D_{a,\mu\nu}\right)|\mu\rangle\langle\nu| = \sum_{\mu}\sum_{\nu}\Delta_{0a;\mu\nu}|\mu\rangle\langle\nu| \tag{2}$$

where in the SDF expression appear the density *coordinates* matrices[2]: $\mathbf{D}_0 = \left\{D_{0,\mu\nu}\right\}$; $\mathbf{D}_a = \left\{D_{a,\mu\nu}\right\}$.

2.4.2 Minkowski norm

Because the difference function ζ as defined in Eq. (2) has the Minkowski pseudo-norm property: $\langle\zeta\rangle = 0$, this signifies that the tensors of the density coordinates difference $\mathbf{\Delta} = \left\{\Delta_{0a;\mu\nu}\right\}$ and overlap $\mathbf{S} = \left\{S_{\mu\nu} = \langle|\mu\rangle\langle\nu|\rangle\right\}$ act as two orthogonal vectors, a fact which can be written with the convention[3]: $\langle\mathbf{\Delta}*\mathbf{S}\rangle = 0$. In other words, the overlap matrix can be considered orthogonal to the difference of the density coordinates matrices obtained with different procedures under the same basis set for the same state.

2.4.3 Euclidian norm

On the other hand, the Euclidian norm of the difference function ζ, which is coincident with the squared Euclidian distance as commented before, will produce a positive definite real number:

$$\langle|\zeta|^2\rangle = \sum_{\mu}\sum_{\nu}\sum_{\lambda}\sum_{\sigma}\Delta_{0a;\mu\nu}\Delta_{0a;\lambda\sigma}\langle\mu\nu\lambda\sigma\rangle\,.$$

[2] The term *density coordinates matrix* is used after the definition of this terminology [36] and for the first time here to avoid confusion. The current literature uses the shorter name *density matrix* instead. However, this latter name is ambiguous, as it is also used in reference to some functional aspect related with the possible matrix-like structure which can be associated to the DF.

[3] The symbol: $\langle\mathbf{A}*\mathbf{B}\rangle = \sum_I\sum_J A_{IJ}B_{IJ}$, meaning the complete sum of an inward matrix (or tensor) product is used here. For more details see [37].

2.4.4 Cioslowski's similarity approach

In a simplified computation of the above Euclidian norm, as Cioslowski suggested [35], the following possible expression can be set up:

$$\begin{aligned}\langle|\zeta|^2\rangle_C &= \sum_\mu \sum_\nu \sum_\lambda \sum_\sigma \Delta_{0a;\mu\nu}\Delta_{0a;\lambda\sigma} S_{\mu\sigma} S_{\lambda\nu} \\ &= \sum_\nu \sum_\sigma \left(\sum_\mu \Delta_{0a;\mu\nu} S_{\mu\sigma}\right)\left(\sum_\lambda \Delta_{0a;\lambda\sigma} S_{\lambda\nu}\right) \\ &= \sum_\nu \sum_\sigma T_{0a;\nu\sigma} T_{0a;\sigma\nu} = \left\langle \mathbf{T}_{0a} * \mathbf{T}_{0a}^T \right\rangle\end{aligned}$$

which produces a final result corresponding to the Euclidian norm of the matrix:

$$\mathbf{T}_{0a} = \left\{ T_{0a;\nu\sigma} = \sum_\mu \Delta_{0a;\mu\nu} S_{\mu\sigma} \right\}.$$

Such a result proves Cioslowski procedure cannot be associated to a clear similarity–dissimilarity index, but just to a scalar product of a matrix by itself, that is: a Euclidian norm.

2.4.5 Centroid shift of an arbitrary set of DF

Given an arbitrary cardinality set of DF: $\mathbb{P} = \{\rho_I \,|I = 1, N\}$ one can always define a centroid DF, just averaging the elements of $\mathbb{P}$:

$$\rho_C = N^{-1} \sum_I \rho_I \rightarrow \langle \rho_C \rangle = N^{-1} \sum_I \langle \rho_I \rangle = N^{-1} \sum_I v_I = v_C$$

Then, the set $\mathbb{P}$ can be origin shifted with respect the above defined centroid DF:

$$\forall I : \zeta_I = \rho_I - \rho_C \rightarrow \mathbb{Z} = \{\zeta_I \,|I = 1, N\}$$

producing the set $\mathbb{Z}$ made of SDF. Then it can also be written:

$$\begin{aligned}\forall I : \zeta_I &= \left(1 - N^{-1}\right) \rho_I - N^{-1} \sum_{J \neq I} \rho_J = N^{-1} \left((N-1)\, \rho_I - \sum_{J \neq I} \rho_J \right) \\ &= N^{-1} \left(N \rho_I - \sum_J \rho_J \right) = N^{-1} \left(N \rho_I - \rho_C \right).\end{aligned}$$

Such a result shows that every centroid SDF corresponds to the averaged difference between each DF in $\mathbb{P}$ repeated N times and the centroid DF. In fact, the selfsimilarity

of every centroid SDF corresponds to the mean squared Euclidian distance between the connected DF and the centroid DF. That is:

$$\forall I : \langle |\zeta_I|^2 \rangle = N^{-2}\left(N^2 \langle |\rho_I|^2 \rangle - 2N \sum_J \langle \rho_I \rho_J \rangle + \sum_J \sum_K \langle \rho_J \rho_K \rangle \right)$$
$$= N^{-2}\left(N^2 Z_{II} - 2N \sum_J Z_{IJ} + \sum_J \sum_K Z_{JK} \right)$$

which is an expression attached to the elements of the set $\mathbb{P}$ where the elements of the overlap similarity matrix appear naturally:

$$\mathbf{Z} = \{ Z_{IJ} = \langle \rho_I \rho_J \rangle \, | I, J = 1, N \}.$$

3 Hohenberg–Kohn theorem

In order to connect the DF origin shift mathematical structure with HKT, previous work about a formulation of the theorem has to be remembered [14]. In this reference the basic notions which will be used here are already developed and demonstrated, so they will be not repeated.

Now, suppose that ρ_0 is the exact DF for the non-degenerate ground state of some Hamiltonian operator H. That is, one can write the expectation value expression for the attached ground state energy as:

$$\langle H \rho_0 \rangle = E_0.$$

At the same time, if ρ_a corresponds to an approximation of the exact DF: ρ_0, then it can be also written:

$$\begin{aligned} \langle H \rho_a \rangle = E_a &\rightarrow E_a \geq E_0 \rightarrow E_a - E_0 \geq 0 \\ &\rightarrow \langle H \rho_a \rangle - \langle H \rho_0 \rangle \geq 0 \rightarrow \langle H \left(\rho_a - \rho_0 \right) \rangle \geq 0 \\ &\rightarrow \langle H \zeta \rangle \geq 0 \leftrightarrow - \langle H \zeta \rangle \leq 0. \end{aligned} \tag{3}$$

Therefore, as a consequence of the variational principle, it can be said that any SDF ζ, involving the approximate-exact pair of considered DF will yield a positive Hamiltonian expectation value.

The same can be said, when the approximate DF ρ_a is considered an exact DF of some Hamiltonian: H_a, providing the energy: $\langle H_a \rho_a \rangle = E_a$. It will be obtained in the same way as before; shifting now the approximate DF ρ_0, with ρ_a which can be now considered that it will act as the exact DF:

$$\begin{aligned} \langle H_a \rho_0 \rangle = E_0^a &\rightarrow E_0^a \geq E_a \rightarrow E_0^a - E_a \geq 0 \\ &\rightarrow \langle H_a \rho_0 \rangle - \langle H_a \rho_a \rangle \geq 0 \rightarrow \langle H_a \left(\rho_0 - \rho_a \right) \rangle \geq 0 \\ &\rightarrow \langle H_a \left(-\zeta \right) \rangle \geq 0 \leftrightarrow \langle H_a \zeta \rangle \leq 0. \end{aligned}$$

A resulting expression which can be trivially summed up to the previous outcome in Eq. (3) to yield:

$$\langle (H - H_a)\, \zeta \rangle \geq 0 \tag{4}$$

or alternatively:

$$\langle (H_a - H)\, \zeta \rangle \leq 0.$$

Therefore, the Hamiltonian operator difference provides a definite non- negative or non-positive expectation value with respect to the SDF. This result must be obtained with an appropriate SDF difference order, inverted with respect to the involved Hamiltonian difference.

This can be easily demonstrated, because the expectation value non-negative property is invariant, upon reversing the DF origin shift and the Hamiltonian orders in the implied differences, that is:

$$\langle (H - H_a)\, \zeta \rangle \geq 0 \rightarrow \langle (H_a - H)\, (-\zeta) \rangle \geq 0.$$

The Hamiltonian differences, appearing at the same time than the DF origin shifts, might be considered as Hamiltonian operator origin shifts too. Thus, origin shift with respect the systems 0 or a, performed in both Hamiltonians and DF, produce the same non-negative or non-positive expectation value characteristic.

Formally, this general expectation value property constitutes the statement of a generalized HKT. Formulated in this way though, HKT might also be simply considered as a consequence of the variational principle. Perhaps because of this general variational connection, the well-known HKT could be renamed as a HK *principle*.

3.1 Extension of HKT

More than an extension, the following property, which will be now discussed, might be seen as related to the HKT itself and thus it could be used as an argument leading to it. Indeed, as it has already been shown in the previous paragraph, suppose first that ρ_0 is the exact DF for the non-degenerate ground state of some Hamiltonian operator H. That is, one can write the expectation value expression for the attached ground state energy as: $\langle H\rho_0 \rangle = E_0$.

At the same time, if $\mathbb{A} = \left\{\rho_I^a\right\}$ corresponds to a set of approximations of the exact DF: ρ_0, then it can be written:

$$\begin{aligned} \forall I : \left\langle H\rho_I^a \right\rangle = E_I^a \rightarrow E_I^a \geq E_0 \rightarrow E_I^a - E_0 \geq 0 \\ \rightarrow \left\langle H\rho_I^a \right\rangle - \langle H\rho_0 \rangle \geq 0 \rightarrow \left\langle H\left(\rho_I^a - \rho_0\right) \right\rangle \geq 0 \rightarrow \langle H\zeta_I \rangle \geq 0. \end{aligned} \tag{5}$$

Because of this property of the SDF, and knowing any convex number set: $K = \{\kappa_I\} \rightarrow \sum_I \kappa_I = 1 \wedge \forall I : \kappa_I \in R^+$ then one can write a convex linear combination

yielding a non-negative result under the considered Hamiltonian:

$$\zeta = \sum_I \kappa_I \zeta_I \rightarrow \langle H\zeta \rangle = \sum_I \kappa_I \langle H\zeta_I \rangle = \sum_I \kappa_I \left(E_I^a - E_0\right) \geq 0.$$

This last sum in the above result can be considered as an average of the energy positive differences:

$$\begin{aligned} \langle \Delta E \rangle &= \sum_I \kappa_I \left(E_I^a - E_0\right) = \sum_I \kappa_I \Delta E_I \\ &= \sum_I \kappa_I E_I^a - \left(\sum_I \kappa_I\right) E_0 = \sum_I \kappa_I E_I^a - E_0 = \left\langle E^a \right\rangle - E_0 \geq 0. \end{aligned} \tag{6}$$

Therefore, even considering an arbitrary number of convex combinations of an approximate DF set, the meaning of the property associated to Eq. (6) is such that, the approximate energy obtained as an expectation value of the exact Hamiltonian will be in any case situated above the exact energy. This result constitutes a clear reformulation of the variational principle.

If the approximate DF set $\mathbb{A} = \left\{\rho_I^a\right\}$ with respect to some Hamiltonian H corresponds to the exact DF for some attached Hamiltonian set:

$$\mathbb{H} = \left\{H_I^a\right\} \rightarrow \forall I : \left\langle H_I^a \rho_I^a \right\rangle = E_I^a,$$

then one can use the approximate energies obtained with the Hamiltonian set $\mathbb{H}$ acting on the original DF ρ_0 :

$$\begin{aligned} \forall I : \left\langle H_I^a \rho_0 \right\rangle = E_{0I} \rightarrow E_{0I} - E_I^a &= \left\langle H_I^a \rho_0 - H_I^a \rho_I^a \right\rangle \\ &= \left\langle H_I^a \left(\rho_0 - \rho_I^a\right) \right\rangle = \left\langle H_I^a \left(-\zeta_I\right) \right\rangle \geq 0. \end{aligned}$$

Then, summing up this final relation with the previous result provided by Eq. (5), it is obtained:

$$\forall I : \left\langle H_I^a \left(-\zeta_I\right) \right\rangle + \langle H\zeta_I \rangle = \left\langle \left(H - H_I^a\right) \zeta_I \right\rangle = \left\langle \left(H - H_I^a\right) \left(\rho_I^a - \rho_0\right) \right\rangle \geq 0$$

proving that the HKT is fulfilled by all the approximate DF, which in turn are the exact DF of some well-defined Hamiltonian set. In fact, this relation which holds for any approximate DF, can be considered a generalization of the previous result, as provided in Eq. (4).

4 Extended variational principle and expectation values ordering

The variational principle might be made extensive to other properties associated to different Hermitian operators other than Hamiltonians.

To evidence this, suppose that a set of exact DF for some system is known and symbolized as: $\mathbb{P} = \{\rho_I \,|I = 0, \ldots N \ldots\}$. Suppose it is also known an Hermitian

operator: Ω, which acting upon the DF set $\mathbb{P}$ produces the set of exact expectation values:

$$\forall I : \langle \Omega \rho_I \rangle = \omega_I. \tag{7}$$

One can freely choose the arbitrary order of the DF, according to the expectation value set (7) ordering, which in turn can be written in such a way that the following inequality sequence holds:

$$\omega_0 \leq \omega_1 \leq \omega_2 \cdots \leq \omega_N \leq \cdots$$

Now, an approximate DF for the lower expectation value might be represented as a convex combination of the exact DF set elements:

$$\rho_a \approx \sum_{I=0}^{N} \alpha_I \rho_I + O\left(N+1\right) \leftarrow \sum_{I=0}^{N} \alpha_I = 1 \wedge \forall I : \alpha_I \in \mathrm{R}^{+}.$$

Then, it can be also employed the fact that the first convex coefficient can be written as:

$$\alpha_0 = 1 - \sum_{I=1}^{N} \alpha_I$$

and rewriting the approximate DF accordingly, while renaming the SDF as has been done before, it is obtained:

$$\rho_a = \rho_0 + \sum_{I=1}^{N} \left(\alpha_I \zeta_I\right) \leftarrow \forall I : \zeta_I = \rho_I - \rho_0,$$

which is a result meaning that one can now define an approximate SDF attached to the minimal expectation value by means of the linear combination:

$$\zeta_a = \sum_{I=1}^{N} \alpha_I \zeta_I.$$

So, in this way nothing prevents that it can be also written:

$$\langle \Omega \zeta_a \rangle = \omega_a - \omega_0 = \sum_{I=1}^{N} \alpha_I \langle \Omega \zeta_I \rangle = \sum_{I=1}^{N} \alpha_I \left(\omega_I - \omega_0\right) \geq 0 \rightarrow \omega_a \geq \omega_0.$$

This last result can be associated in turn to the following meaning. Considering first for some system its exact DF set has been ordered according to the ascending values of some exact expectation value sequence of some Hermitian operator. Then, as a

consequence, any approximation to the minimal expectation value becomes always an upper bound of the minimal exact one.

Therefore, a sort of variational principle can be set up for the expectation values of any Hermitian operator.

In fact, as another facet of this general property, the variational principle, attached to the ground state energy, can be considered as an intrinsic property of the energy eigenvalues ordering, based on thermodynamical stability considerations.

Such ordering property, involving any Hermitian operator, which has been previously disclosed here, might be named as an *extended* variational principle.

5 The extended HK principle

If the variational principle could be generalized according to the ordering of any expectation value, under some particular circumstances, then the HK principle can be extended to some Hermitian operator. Suppose the ascending order of the DF set is performed according to the expectation values of some Hermitian operator Ω, as discussed in the previous paragraph. Then it can be written:

$$\langle \Omega \rho_0 \rangle = \omega_0.$$

At the same time, if ρ_a corresponds to an approximation of the exact DF then it can be also written:

$$\begin{aligned} \langle \Omega \rho_a \rangle = \omega_a \rightarrow \omega_0 \leq \omega_a \rightarrow \omega_a - \omega_0 \geq 0 \\ \rightarrow \langle \Omega \rho_a \rangle - \langle \Omega \rho_0 \rangle \geq 0 \rightarrow \langle \Omega \left(\rho_a - \rho_0 \right) \rangle \geq 0 \rightarrow \langle \Omega \zeta \rangle \geq 0. \end{aligned}$$

The same can be said, when the approximate DF ρ_a is considered an exact DF of some Hamiltonian: H_a, say, which can be attached in turn to another Hermitian operator Ω_a. It will be obtained now, in the same way as before:

$$\langle \Omega_a \left(-\zeta \right) \rangle = \langle \Omega_a \left(\rho_0 - \rho_a \right) \rangle = \omega_a^0 - \omega_a \leq 0 \leftarrow \omega_a \leq \omega_a^0,$$

which can be rewritten as: $-\langle \Omega_a \left(\rho_a - \rho_0 \right) \rangle = -\langle \Omega_a \zeta \rangle \geq 0$ and can be trivially summed up with the previous result to yield:

$$\langle \left(\Omega - \Omega_a \right) \zeta \rangle \geq 0.$$

Of course, in order to arrive at the same conclusion as the one reached considering the system energies within HK principle, the operator difference: $\Omega - \Omega_a$ has also to be constructed as different from the zero or null operator.

In this way and under the obvious restrictions already mentioned, one can consider the HK principle to hold in some specific manner for any Hermitian operator expectation values.

6 Conclusions

Origin shifts performed within DF sets can be considered as some kind of basic building block to demonstrate the HKT. In doing so, the HKT appears as a consequence of the variational principle. Thus, perhaps one can speak in a more general way about the HK principle too.

Moreover, origin shifts implemented within DF sets, permit to generalize the variational principle, whenever a Hermitian operator is considered and the DF order follows a new ordering, related to the associated expectation values of such an operator. Then, this extended variational principle induces a possible generalization of the HK principle, whenever two distinct Hermitian operators can be defined for the exact and approximate DF.

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