

# A Derivation of Quantum Mechanics from START

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Quantum Mechanics is a successful model to describe physical phenomena. We show that a simple set of postulates about the description of objects in Nature allows the derivation of the principles of QM, transforming this theory into a deductive approach to Physics. The main postulate is: Objects are described as energy distributions in Space–Time.

## 1 Quantum Mechanics from START

It is universally accepted that Quantum Mechanics is a successful model to describe physical phenomena, in particular of the electronic structure of atoms, molecules and solids. As such it has been reformulated in several different forms (see for example: *Nine formulations of quantum mechanics*, Daniel F. Styer et al. [15]). The aim of the present paper is to show that a simple set of postulates about the description of objects in Nature allows the derivation of the principles of QM, transforming this theory into a deductive approach to Physics. In our approach the main postulate is: Objects are described as energy distributions in Space–Time. The theory is in fact a systematic mathematical analysis of this postulate and of other general considerations about action, energy–momentum and the role of the theory as a useful description of Nature.

The paper also shows the fundamental and basic status of Density Functional Theory, also contained in our approach.

The initial mathematical structure is a geometric (quadratic form based) union of space, time and action. In physics bundles of trajectories are used to describe the objects of nature: distribution of heights over a surface, a real object is described as a bundle of space-time trajectories, here we use a description as a bundle of action valves in space-time (energy densities in space following light-like lines).

The author is fully aware that the presentation is strongly guided by the knowledge of the usual computational approach to study atoms, molecules and condensed matter electronic structure.

### 1.1 The quadratic form in physics

Formally our approach, a Space–Time–Action Relativity Theory: START [9, 10], represents the physical world as a 5-D continuum with a quadratic form. Historically the initial use of a quadratic form  $l^2 = x^2 + y^2 + z^2$  to describe nature came with the now known as Pythagoras Theorem, which even today is geometrically used in 3-D statics studies. At the beginning of the XXth century the 4th dimension was added in the Minkowski  $s^2 = (ct)^2 - l^2$  space-time formalism. For our purpose we consider also a distribution of an action variable  $w = \kappa_{(0)}\bar{a}$ ,  $\kappa_{(0)} = \frac{d_{(0)}}{h} = \frac{c}{E_{(0)}}$ ,  $(\bar{a})^2 = \sum_{\mu} a_{\mu}^2$ ;  $\mu = 0, 1, 2, 3$  over space-time  $h$  being Planck's constant and  $d_{(0)}$

a system's fundamental length. This is schematically shown in the next table

| From Pythagoras to the XXIst Century     |                        |                    |
|--|------------------------|--------------------|
| Quadratic Form                           | Dim/diff. Op           | Group              |
| $l^2 = x^2 + y^2 + z^2 \quad (\Delta t)$ | 3-D $\nabla, \nabla^2$ | Statics, Galileo   |
| $s^2 = (ct)^2 - (x^2 + y^2 + z^2)$       | 4-D $D, \square^2$     | Kinetics, Poincaré |
| $S^2 = (ct)^2 - (x^2 + y^2 + z^2) - w^2$ | 5-D $K, \diamond^2$    | Dynamics, START    |

In this geometrical setup we use a 5-D Relativity Principle “**For physical systems all trajectories are null for all observers**”. Within the geometry, to obtain a comprehensive theory, the development of the theory follows:

| The Geometrical Structures of Physics                          |                          |                |
|--|--------------------------|----------------|
| SPACE + TIME + ACTION  |                          |                |
| +  |                          |                |
| Fundamental <b>Principles</b> and <b>Postulates</b> (Carriers) |                          |                |
| ↓  |                          |                |
| START Geometry   |                          |                |
| ↙  | ↓                        | ↘              |
| General Relativity   | <b>Quantum Mechanics</b> | Standard Model |

In this program:

- **Principles** refer to primitive concepts and relations as, for example, the existence of a unified geometry for space, time and action.
- **Postulates**, to complementary concepts as the geometrical union of the manifold of those variables through the use of two constants universal  $c$  and  $\kappa_0$ , generating the geometry we have called START, a quadratic space.
- For a given observer the physical objects constituents of a system are the **carriers**, defined as a distribution of energy over space  $E_{(c)}(x, t) = \varepsilon_{(c)}\rho_{(c)}(x, t)$ , where  $\varepsilon_{(c)}$  is the energy per equivalent carrier of type  $c$ .
- Two basic additional principles introduce the **unit of action**  $h$  in relation to the amount of action that can be given or taken from a system (usually described as energy and angular momentum being exchanged, this is tautologically the definition of a system) and to a **freedom of description** of matter within START.

## 1.2 Hypothesis and principles in START

Physics is the science which describes the basic phenomena of Nature within the procedures of the Scientific Method. The mathematization of the anthropocentric, primary, concepts of space, time and the existence of the physical objects (action **carriers**), is a suitable point of departure for creating intellectual structures which describe Nature.

We have introduced a set of principles [12, 9, 10]:

**Relativity**, complex Poincaré group and complex Lorentz transformations.

**Existence**, physical objects are represented by energy densities.

**Least Action**, (null trajectories in START).

**Quantized Exchange of Action**, defines systems or subsystems as those among a quanta of action can be exchanged.

**Choice of Descriptions**, allows all useful physical models to be employed.

From this we derive, in this and in previous papers, some of, the fundamental structures of Physics.

### 1.3 Derivation of the structure of Quantum Mechanics

The formal steps to be followed, schematically presented here, are

| Steps            | Subject  | Formal Relation   |
|------------------|--|---|
| 1a define        | Action Density in Space-Time                   | $a(X) \rightarrow E(x, t)$  |
| 1b equivalent to | Energy Density in Space                        | $E(x, t) = \sum^{(c)} E_{(c)}(x, t)$                                    |
| 2 using a        | Definition of (equivalent) Carriers            | $E_{(c)}(x, t) = \epsilon_{(c)} \rho_{(c)}(x, t)$                       |
| 3 and the        | Energy-Momentum condition                      | $p_\mu \doteq \partial_\mu a(X)$  |
| 4a imposing an   | Analyticity requirement                        | $\rho_{(c)}(x, t) = \Psi^\dagger(x, t)\Psi(x, t)$                       |
| 4b also          | Least Action requirement: $\square^2 \Psi = 0$ | $\gamma_4 \hbar K \Psi = 0 \rightarrow i \hbar \partial \Psi = mc \Psi$ |
| 5 with a         | Gauging and Description Choice                 | $\Psi \rightarrow \Psi \exp(i\phi(X))$                                  |

That is matter is considered a (time-dependent) distribution of energy in space as a summation among carriers. Equivalent carriers in a system are attributed by definition the same amount of energy per carrier. If a different amount of energy has to be attributed to two, otherwise considered identical, carriers then they are not equivalent. Energy-momentum is defined as the rate of change of action. The finiteness of the amount of matter and the corresponding energy require that action and then the density obey analytical conditions, to fulfil this condition, as shown below (Keller and Weinberger [11]), the density has to be written as a product of the corresponding pair of square integrable analytical functions. In order to obtain the least action state we follow the Schrödinger procedure (Schrödinger 1926 [14]) to optimize the total action variable functional, which produces the wave equation. Finally because of the analyticity requirement the auxiliary amplitude functions are only defined up to general multivector phase factor  $s$ :

$$\phi = \sum^{\text{multivectors } A} \phi_A \gamma^A \quad \text{scalar, vector, bivector, etc.} \quad \text{then} \quad i \hbar \partial \Psi^\circ = mc \Psi^\circ + \overrightarrow{\Delta V} \Psi^\circ.$$

The energy (action) carriers can be given specific names according to the mathematical structure of the corresponding densities. The words simple and composite referring to one term or several terms, the word decomposable to the fact that each of the terms is proportional to one given density (as in the case of equivalent electrons in atomic, molecular, and solid state structure). Because we can use for the description an average description, we can either define the average carrier or an average description. In most cases we are in fact using the definition of the carrier in a system through the introduction of some effective potential acting upon it. Then, as this kind of carrier can not be studied in the absence of that potential, we should really call that carrier a pseudo-carrier. This is summarized

| Classification of Carriers           |   |
|--------------------------------------|---|
| Carrier Type                         | Description Type  |
| Elementary (Simple)                  | $\rho_C(\mathbf{x}, t) = \rho_c(\mathbf{x}, t)$   |
| Elementary (Composite)               | $\rho_C(\mathbf{x}, t) = \sum_c A^c \rho_c^{\{c \in C\}}(\mathbf{x}, t)$  |
| Decomposable                         | $\rho_C(\mathbf{x}, t) = n^D \rho_D(\mathbf{x}, t)$   |
| Average Carrier                      | $\rho_A(\mathbf{x}, t) = \frac{1}{W} \sum_{c=1}^N A^c \rho_c(\mathbf{x}, t)$  |
| Description Average ( $\bar{\rho}$ ) | $\rho_C(\mathbf{x}, t) = \frac{1}{W} \sum_{c=1}^N \frac{1}{\tau} \int_{\lambda=\lambda_0}^{\lambda=\lambda_0+\tau} A^c(\lambda) \rho_c(\mathbf{x}, t) d\lambda$ |
| Pseudo-Carriers                      | $\{\rho_c(\mathbf{x}, t)\} \rightarrow \rho_C^{\text{eff}}(\mathbf{x}, t) \quad [V_{\text{eff}}]$   |

With corresponding definitions of averaging weights and auxiliary amplitude functions:

|   |   |
|---|---|
| $W = \sum_{c=1}^N A^c$  | $\bar{W} = \sum_{c=1}^N \frac{1}{\tau} \int_{\lambda=\lambda_0}^{\lambda=\lambda_0+\tau} A^c(\lambda) d\lambda = 1$ |
| $\Psi = \sum_l \mathbf{a}_l \sum_m \mathbf{p}_m \prod_s \phi_s^{\{l,m\}}$ | $\phi_s^{\{l,m\}} = \sum b_n \prod \phi_\beta^{(n)}$  |

## 2 The density

We come back to the conditions to be obeyed by the analytical function  $\rho_c(\mathbf{x}, t)$ .

- D1.  $\rho_c(\mathbf{x}, t)$  is a real quantity  $\rho_c(\mathbf{x}, t) \in \mathbb{R}$ .
- D2. The density  $0 \leq \rho_c(\mathbf{x}, t) < \infty$  in order to represent a finite amount of action.
- D3. The derivatives of the density  $-\infty < \partial_\mu \rho_c(\mathbf{x}, t) < +\infty$  in order to represent a finite amount of energy–momentum.
- D4. The integral of the density  $\int_{\Omega_C} \rho_c(\mathbf{x}, t) d\Omega = n$  in the  $n$  carriers' volume  $\Omega_c$ .

**Theorem 1 (Keller and Weinberger 2002).** *If  $\Psi(x, t)$  is an analytical quadratic integrable complex or multivector function, conditions D1, D2 and D3 are fulfilled identically if  $\rho_c(x, t) = |\Psi_c(\mathbf{x}, t)|^2$ . Here  $|f|^2$  means the real quadratic form of any more general function  $f$ , even if  $f$  itself is not necessarily a real function and we define: if  $|f|^2 = f^+ f$  then  $\partial_\mu |f|^2 = (\partial_\mu f^+) f + f^+ (\partial_\mu f)$ .*

**Proof.** **Reality** condition D1 is fulfilled by the definition  $\rho_c(\mathbf{x}, t) = |\Psi_c(\mathbf{x}, t)|^2$ , **Carrier Finiteness** D2 by the requirement of quadratic integrability, **Energy Finiteness** D3 by the definition  $\partial_\mu |f|^2 = (\partial_\mu f^+) f + f^+ (\partial_\mu f)$  and the analytical properties of  $\Psi(\mathbf{x}, t)$ . ■

It can be seen that the conditions D1, D2, D3 and **normalization**  $\int_V \rho_c(\mathbf{x}, t) d\mathbf{x} = n_c$  correspond to the  $\Psi(\mathbf{x}, t)$  being quadratic integrable **Hilbert functions**. In any Lagrangian type formulation this last definition of  $\rho$  can be used as a condition introduced via a Lagrange multiplier.

### 2.1 The auxiliary amplitude function

There is an additional number of conditions that the auxiliary amplitude function will have to fulfil in order to be adequate to describe different physical situations and systems as discussed below. Besides conditions of purely mathematical origin there will be additional conditions from physical considerations about the system to be described. There are two main ones.

First the description of **alternate possibilities**  $\phi_s^{\{l,m\}} = \sum^i a_i \varphi_i^{(S)}$  which are to be included together in the formulation, alternatives which can be either of fundamental physical origin or arising from the choice of describing a system with several alternatives without the selection of only one set of alternatives. This first choice will immediately be related to concepts of either statistics of probabilities in the measurement. That is if an actual measurement will be performed, some statistical distributions would be found. Probabilistic in the sense that if an actual measurement is performed one or one set of states would be found with an attached probability. It is fundamental to distinguish between statistics referred to actual distributions and probabilities referred to possible outcomes of a measurement. Second, the fact that many systems are better described, or should in fact be described, as collections of “carriers” introduces an additional condition which is also called “statistics”: the carriers can be equivalent or non-equivalent and in the case of equivalent carriers the descriptions of some carriers of the system can be the same as the description of others (the so-called Bose–Einstein statistics) or alternatively should be all different (the so-called Fermi–Dirac statistics). In the case of the Fermi–Dirac statistics the auxiliary amplitude function must mathematically be built from a combination of at least as many, in the Hilbert function sense, orthogonal functions as there are equivalent carriers to be described.

In the 77 years during which quantum mechanics has been under construction it has been useful to introduce names related to the functions, as for example: basis functions, basis sets, states, configurations, etc. and the every use day of these names can sometimes be felt as corresponding to physical entities and not just to the elements of a mathematical description. This is even more the case because the symmetries relating these mathematical elements and other properties of the solutions of the differential equations obeyed by the functions are in themselves useful to analyze experimental results.

## 2.2 The geometry of the auxiliary amplitude functions

In the case of a relativistic treatment of the optimization procedure to obtain the least action state we have to include a geometrical Lorentz transformation  $R(x)$ . This (as discussed in Keller [7]) corresponds to a transformation of the energy-momentum 4-vector  $p_\mu$  followed by the procedure of obtaining the components from the auxiliary amplitude functions, as follows

| Algebraic Equation for the Amplitude Function (Keller 1991)   |                           |
|---|---------------------------|
| $e_\mu p^\mu(\mathbf{x}), \quad \mathbf{x} = e_\mu x^\mu$   | $p^\mu$ per unit $\rho$   |
| $e_\mu p^\mu(\mathbf{x}) = p^{(0)} e_0^{(0)} \quad (1)$   | Lorentz Transf.           |
| $e_\mu^{(0)} = R(\mathbf{x}) e_\mu R^{-1}(\mathbf{x}), \quad R^{-1} = R^\dagger$  | Lorentz Transf.           |
| $e_\mu p^\mu(\mathbf{x}) = p^{(0)} R(\mathbf{x}) e_0 R^{-1}(\mathbf{x}) \quad (2)$  | Lorentz Transf.           |
| $e_\mu p^\mu(\mathbf{x}) R(\mathbf{x}) = p^{(0)} R(\mathbf{x}) e_0 = m_0 c R(\mathbf{x}) e_0,$  | $R(\mathbf{x})$ on right  |
| $P_{+\uparrow} = e_0 P_{+\uparrow} = P_{+\uparrow} e_0, \quad P_{+\uparrow} = P_{+\uparrow} i e_1 e_2$                                | Ref. Projectors           |
| $e_\mu p^\mu R(\mathbf{x}) P_{+\uparrow} = m_0 c R(\mathbf{x}) P_{+\uparrow} i e_0 e_1 e_2, \quad (3)$                                | Apply Projectors          |
| $\Psi(\mathbf{x}) = A(\mathbf{x}) R(\mathbf{x}) P_{+\uparrow} \in \widehat{C}_{1,3}, \quad (4)$                                       | Square Root of $\rho$     |
| $-i \hbar \partial^\mu e_\mu \Psi(\mathbf{x}) = m_0 c \Psi(\mathbf{x}) i e_0 e_1 e_2 = \hbar \partial^4 \Psi(\mathbf{x}) e_0 e_1 e_2$ | $\Psi(\mathbf{x})$ in (3) |
| $\rho = \rho(\mathbf{x}) = A^2(\mathbf{x}),$  | Define Density            |
| $\rho = j^0 = \Psi(\mathbf{x}) e_0 (\Psi(\mathbf{x}))^\dagger,$   | Carrier Density           |

The function  $\Psi(\mathbf{x}) = \Psi^V(\mathbf{x})$  above explicitly contains then three main contributions: the **existence of the carriers’** field in  $A^V(\mathbf{x})$ ; the observer’s description of the **relative motion**

**of the field** in  $R(\mathbf{x})$  a (local) Lorentz transformation; and the reference to a **preferred sign of rest mass**  $m_0$  and, writing  $R(\mathbf{x}) = R^V(\mathbf{x})R^{(0)}$  **spin** (through  $R^{(0)}$  and  $P_{+\uparrow}$ ). The density  $\rho(\mathbf{x}) = j^0(\mathbf{x})$  must be an acceptable density in the presence of the external potential  $V(\mathbf{x})$ .

As mentioned the formal structure of quantum mechanics allows a statistical analysis of both the structure of the density and the structure of the amplitude functions. This is as far as in probability theory a normalized summation of probabilities corresponds to alternatives in the outcome of the statistical study and a product of probabilities to sequential conditions in the statistical analysis. The amplitude functions can then be written as sums of products:

| <b>“Probability” in the Derivation of Quantum Mechanics from START</b>  |  |
|---|--|
| $\Psi^S = \sum_{l=1}^L \mathbf{a}_l \left\{ \sum_{m=1}^m \mathbf{p}_m^{(l)} \prod_{s=1}^n \phi_s^{\{l,m\}} \right\}$  | $\phi_s^{\{l,m\}} = \sum_i^i a_i \varphi_i^{(S)}$  |
| Sum of $L$ Descriptions of $n$ Carriers<br>$\Psi^S =$ Linear Form of $\rho$ (quadratic scalar)<br>$ \mathbf{a}_l ^2 \Rightarrow$ weight of collective description | $\phi_s^{\{l,m\}}$ <b>describes</b> 1 carrier in S<br>$ a_i ^2 \Rightarrow$ weight of basis description<br>$\left\{ \sum_{m=1}^m \mathbf{p}_m^{(l)} \prod_{s=1}^n \phi_s^{\{l,m\}} \right\} \Rightarrow \mathbf{n}$ carriers |

### 3 KKW-DFT

We proceed now to the specific analysis corresponding to density functional theory [13]. The result is that the theorems of Hohenberg and Kohn [2] and of the present author and collaborators appear now as basic natural conditions in the logical structure of the theory [3–6]. Our initial approach is not related with the replacement of the local study of the properties of the density with those of an equivalent density of a gas of carriers (free electron gas for example).

From the considerations above we describe each and any of the  $n$  carriers obeying Fermi–Dirac statistics through an auxiliary amplitude function  $\psi_i = \phi_s^{\{l,m\}}$  (describing carriers in the system  $S$ ) where  $\langle \psi_i \psi_j \rangle = \delta_{ij}$ , then

$$\psi_i = \sum_{\lambda} a_i^{\lambda} \varphi_{\lambda}, \quad \sum_{\lambda} |a_i^{\lambda}|^2 = l \quad \text{for all } i = 1, \dots, n, \quad \text{where } \sum_i |a_i^{\lambda}|^2 = w^{\lambda},$$

and the weight of every spin–orbital

$$\sum_{\lambda} w^{\lambda} = n \quad \text{number of electrons, such that } |a_i^{\lambda}|^2 = |a_j^{\lambda}|^2, \quad i, j = 1, \dots, w,$$

according to the requirement that the density descriptions of all carriers are equivalent. That is

$$(a_i^{\lambda})^* a_j^{\lambda} + a_i^{\lambda} (a_j^{\lambda})^* = 2w^{\lambda} \delta_{ij} \quad \text{and} \quad \int \frac{1}{2} (\varphi_{\lambda}^* \varphi_{\mu} + \varphi_{\lambda} \varphi_{\mu}^*) dv = \delta_{\lambda\mu},$$

consequently all  $\varphi_{\lambda}$  should be solutions of the same differential equation corresponding to different eigenvalues. Also we define

$$\int \rho d\text{vol} = n, \quad \rho = \sum_i |\psi_i|^2 = \sum_i \rho_i = n\rho_i = n\rho_{(1)}, \quad \rho_i = \rho_j = \rho_{(1)} \quad \text{all } i, j.$$

With these definitions we can compute the carrier–carrier interaction energy as the sum  $\varepsilon_{c-c} = \varepsilon_{\text{coul}} + \varepsilon_{\text{xc}}$ , where

$$\varepsilon_{\text{coul}} = \frac{(n-1)}{2} \iint \rho(2)\rho(1) \frac{e^2}{r_{12}} dv_2 dv_1, \quad \varepsilon_{\text{xc}} = \sum_s \frac{n}{2} \iint \rho_{(xc)}^s(2)\rho_{(xc)}^s(1) \frac{e^2}{r_{12}} dv_2 dv_1,$$

$$\rho_{xc}^s(x) = \frac{1}{2} \sum_{\lambda\mu} \frac{1}{2} \left[ (a_i^{\lambda})^* a_i^{\mu} \varphi_{\lambda}^*(x) \varphi_{\mu}(x) + a_i^{\lambda} (a_i^{\mu})^* \varphi_{\lambda}(x) \varphi_{\mu}^*(x) \right]^s,$$

where the super-index  $s$  stands for spin.

### 3.1 The Pauli exclusion principle, exchange and correlation

The above formulation of density functional theory includes the crucial concept of carrier statistics in its formulation for a set of carriers, the one corresponding to what, in the standard literature, is called **fermions**. This is, a type of carriers for which, although being indistinguishable, a “exclusion principle” applies stating that “not two identical carriers can be described the same”. That is what is usually called the Exclusion Principle after Wolfgang Pauli’s formulation in 1923. For these type of carriers even if the density per carrier is the same as far as they are indistinguishable, for each carrier there should be a description, through the auxiliary amplitude function, which must be explicitly different.

- Otherwise stated in the case of fermion carriers the formulation of the exclusion principle can not simply be the textbook type: “two equivalent fermion carriers can not occupy the same state” without specifying that nevertheless they are equivalent. Then the concept “different states” in fact has to refer to different mathematical descriptions of “physically equivalent states”. This is in fact present even in the accepted formulation of quantum mechanics where a symmetrization is always performed which renders the carriers equivalent. For example the so-called Hartree–Fock scheme, which after Slater can be synthetically described to that corresponding to a single determinant wave function, is in fact an explicit form of introducing the equivalence of the carriers as a weighted sum of descriptions where every carrier is in turn described as occupying each one of the available “states”. The systematic continuation of the Hartree–Fock scheme through the so called Configuration Interaction is introduced as a weighted sum of Slater determinants, assuring thus that each term describes each carrier as equivalent to the other ones. Then the correct formulation of the Pauli exclusion principle states:
- *The description of each carrier of any pair of equivalent carriers should be different.*

In short for fermion carriers the density distribution of each carrier has to be the same but the auxiliary function for each carrier must be different (and is not necessary different for boson carriers).

In our formulation as above this auxiliary condition demands that the auxiliary function for each of the  $n$  carriers, a sum over  $m \geq n$  descriptions, contains a set of mutually orthogonal coefficients for each description  $\lambda$  where each coefficient squares to the same real number  $w^\lambda/n$ . In our formulation  $m > n$  corresponds to what is called Configuration Interaction.

#### 3.1.1 Exchange distribution density

The considerations for the case of fermion carriers define an additional new kind of distribution function: When the real square of the auxiliary function is taken, to obtain the carrier distribution  $\rho$ , a sum of cross terms  $\rho_{\lambda\lambda'}(x)$  is also obtained. Each individual term  $\rho_{\lambda\lambda'}(x)$  integrate to zero, also their sum.

This sum  $\rho_{(X)} = \sum_{\lambda\lambda'} \rho_{\lambda\lambda'}(x)$  defines anyhow a new kind of distribution density where two auxiliary description functions are multiplied together, which we will call Exchange Distribution Density. Below these terms contribute to the evaluation of the pair wise interaction energy which corresponds to what is usually denoted as exchange and correlation energy. Then the additional contributions can be summed into two different terms, first, from the usual concept of exchange energy, a sum over  $n$  terms with coefficient  $1/n$  and the rest of the terms corresponding to the usual concept of correlation contribution.

Then our formulation includes all customary descriptions of the energy contributions in an explicit form.

### 3.1.2 The START formulation of the exchange and correlation density functionals and local potentials

The existence of the exchange distribution density allows the direct formulation of the density functional for the exchange–correlation energy and of, through derivation with respect to the density, the local exchange–correlation potentials.

The exchange–correlation energy, as stated above, consists of two parts: the pair wise interaction terms arising from the exchange distribution density (here  $\sum^s$  stands for the two spin values)

$$\varepsilon_{xc} = \sum^s \iint \rho_{xc}(2)\rho_{xc}(1) \frac{e^2}{r_{12}} dv_2 dv_1 = \iint \rho_{xc}(2)\chi(1)\rho(1) \frac{e^2}{r_{12}} dv_2 dv_1,$$

and the self-coulomb part which is, in view of the equivalence of all electrons, the fraction  $-1/n$  of the Coulomb interaction energy arising from the density–density pair-wise interaction (this term is already included above as part of the definition of the correct density–density Coulomb interaction energy)

$$\Delta\varepsilon_{\text{self-coul}} = -\frac{1}{2} \iint \rho(2)\rho(1) \frac{e^2}{r_{12}} dv_2 dv_1,$$

if a comparison is made with the usual approach the two terms above should be added. From these terms the local potential from the exchange–correlation part is directly obtained through a direct functional derivative:

$$V_{xc}^s(1) = \int \rho_{xc}(2)\chi(1) \frac{e^2}{r_{12}} dv_2,$$

where the new variable, *exchange ratio*  $n\chi(x) = 2\rho_{xc}^s(x)/\rho(x)$ , the ratio of the (per spin) exchange density to the total (per spin) local electron density, has been introduced. The equations to solve for the auxiliary functions (central charge  $Ze$  atomic-like calculation) are

$$-\frac{1}{2m} \nabla^2 \psi_i + \left[ -\frac{Ze^2}{r_1} - \left(\frac{n}{2} - 1\right) \int \rho_{xc}(2)\chi(1) \frac{e^2}{r_{12}} dv_2 + (n-1) \int \rho(2) \frac{e^2}{r_{12}} dv_2 \right] \psi_i = \varepsilon_i \psi_i, \quad (1)$$

and the calculation of the total electronic energy

$$E = \sum_i \varepsilon_i - \frac{1}{2} \left[ (n-1) \iint \rho(2)\rho(1) \frac{e^2}{r_{12}} dv_2 dv_1 - \left(\frac{n}{2} - 1\right) \iint \rho_{xc}(2)\chi(1)\rho(1) \frac{e^2}{r_{12}} dv_2 dv_1 \right].$$

As the auxiliary functions corresponding to descriptions of equivalent carriers are a unitary linear transformation ( $a_i^\mu$ ) of a basis set  $\{\varphi_\mu\}$ , the same equation (1) can be used to solve for the basis functions  $\varphi_\mu$ . Also the eigenvalues  $\varepsilon_i$  (the same for the  $\psi_i$ ) can be given in terms of the eigenvalues  $\varepsilon'_\mu$  of the  $\varphi_\mu$  as  $\varepsilon_i = \sum_\mu \|a_i^\mu\|^2 \varepsilon'_\mu$ .

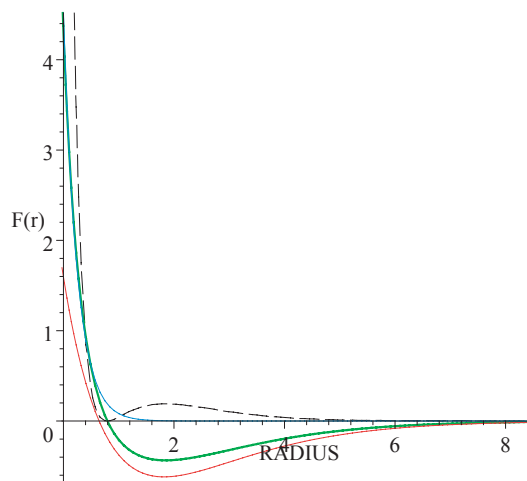
For systems with a small number of electrons the dominant factor is  $((n-1)/n)$  in the electron–electron Coulomb interaction. It is basic for the calculation of the hydrogen atom, it is dominant in the calculation of the Helium atom where each of the two electrons interacts with the other but not with itself, and progressively less important for larger systems where the exchange density and the, to it related, exchange interaction grows.

In the case of the calculation of the Beryllium atom, for example,  $((n-1)/n) = 3/4$  and the exchange density (dotted line), shown in the Fig. 1<sup>1</sup>, is now as important as the basis functions densities. In the same figure (dashed line) the per electron auxiliary function and its components (1s and 2s thin solid lines) are shown as well as the corresponding electron density (dashed line). The relevant energies for Ne, for example, in this case are:

<sup>1</sup>Figures in colour will be available only in electronic version.



| Energy Contribution (Ne atom)                                    | energy (Hartree units) |
|--|------------------------|
| electron-nuclear   | -310.0951              |
| electron-electron coulomb  | 59.20975 (+6.5788)     |
| electron-electron exchange correlation<br>including self-coulomb | -13.2254<br>-6.5788    |
| kinetic energy   | 128.766                |
| total energy (exp. -128.94)                                      | -128.766.              |



**Figure 1.** Beryllium atom exchange density.

The calculation is simple. The same procedure and code to obtain the total density can be used to obtain the exchange density from the same auxiliary functions. The same procedure to obtain the electron–electron coulomb potential and energy is used to obtain the (local) exchange potential and exchange energy. The self-consistent algorithm remains the same. The entire procedure is at least as feasible as the currently employed density functional procedures for actual calculations. In the case of a solid the factor  $f = \lim_{n \rightarrow \infty} ((n - 1)/n) = 1$  is irrelevant and the summation over pairs of basis functions becomes the starting point for the correct description of exchange and correlation. In condensed matter calculation of the double summation over pairs of auxiliary functions should be replaced by actual double integrals.

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