

## FOOTNOTES

### Chapter One.

- <sup>1</sup> The outstanding textbook on TF theory is still P. Gombás, Die statistische Theorie des Atoms und ihre Anwendungen (Springer, Wien, 1949). Then there is the review article N.H.March, Adv.Phys. 6, 1 (1957). A more recent introductory text is N.H.March, Self-consistent Fields in Atoms (Pergamon, Oxford, 1975).
- <sup>2</sup> L.H.Thomas, Proc.Cambridge Phil.Soc. 23, 542 (1926); E.Fermi, Rend. Lincei 6, 602 (1927); D.R.Hartree, Proc.Cambridge Phil.Soc. 24, 89 (1928); V.Fock, Zschr.f.Phys. 61, 126 (1930).
- <sup>3</sup> In the form of a textbook this material has been presented by W. Thirring, Lehrbuch der Mathematischen Physik, Vol.4: Quantenmechanik großer Systeme (Springer, Wien-New York, 1980). A recent review is E.H.Lieb, Rev.Mod.Phys. 53, 603 (1981). A treatment with emphasis on thermal properties is given by J.Messer, Temperature Dependent Thomas-Fermi Theory (Lecture Notes in Physics, Vol.147) (Springer, Berlin-Heidelberg-New York, 1981).
- <sup>4</sup> Models of screened Bohr atoms have been studied to some extent by R.Shakeshaft and L.Spruch, Phys.Rev. A 23, 2118 (1981). Their emphasis is on the oscillatory terms, about which we shall have to say something in Chapter Five.
- <sup>5</sup> This statement is frequently called the Hellmann-Feynman theorem. Both Hellmann (1933) and Feynman (1939), however, only rediscovered what had been known before. It is, indeed, difficult to imagine how quantum mechanics could have been developed without such a central tool. The theorem appears explicitly in Pauli's review of 1933, in Van Vleck's book of 1932, and in a paper by Güttinger in 1931. The latter contains, to my knowledge, the explicit statement for the first time. The various references are: P.Güttinger, Zschr.f.Phys. 73, 169(1931); J.H. Van Vleck, The Theory of Electric and Magnetic Susceptibilities (Oxford University Press, 1932);

W.Pauli, Handbuch der Physik, Vol.24, Part I, p.83, edited by H. Geiger and K.Scheel (Springer, Berlin, 1933); H. Hellmann, Zschr. f.Phys. 85, 180 (1933); R.P.Feynman, Phys.Rev. 56, 340 (1939).

## Chapter Two.

- <sup>1</sup> This is written for the situation of an isolated atom. For applications to molecules and solids, the term  $-Z/r$  has to be replaced by the respective external electrostatic potential. Or, if the atom is part of a gas, an additional term is needed to describe the pressure exerted by the other atoms. If the formalism is being applied to isolated self-binding systems of fermions, like a nucleus with its strong interactions, or a neutron star held together by gravity, the fermion-fermion interaction part is the entire effective potential.
- <sup>2</sup> The potential is not physically unique, because there is the freedom of adding a numerical constant. In writing Eq. (1), we have opted for the usual normalization:  $V \rightarrow 0$  for  $r \rightarrow \infty$ , which means that this constant is set equal to zero.
- <sup>3</sup> Since the potential is subject to the usual normalization  $V(r \rightarrow \infty) = 0$ ,  $\delta V$  has to vanish at infinity. This does, however, not affect the argument, because it suffices to set  $\delta V(\vec{r}) = -\delta\zeta$  for those  $\vec{r}$  for which the density is nonzero.
- <sup>4</sup> The vacuum is not essential; one could, with little additional complications, equally well consider a dielectric surrounding.
- <sup>5</sup> Many applications of this and other, related stationary principles can be found in J.Schwinger's (unfortunately still unpublished) lecture notes on Electromagnetic Theory (University of California, Los Angeles, 1975 ... 1984).
- <sup>6</sup> Strictly speaking, the first equality holds only for nonvanishing density, since  $n=0$  implies no more than  $V+\zeta \geq 0$  in Eq. (51). This subtlety does not affect the argument, however.
- <sup>7</sup> In rewriting  $E_2$ , one has to make use of the identity (the spherical symmetry is essential here)

$$\begin{aligned} [\vec{\nabla} \left( v + \frac{z}{r} \right)]^2 &= \left[ \frac{d}{dr} \left( v + \frac{z}{r} \right) \right]^2 \\ &= \frac{1}{r^2} \left[ \frac{d}{dr} \left( r \left( v + \frac{z}{r} \right) \right) \right]^2 - \frac{1}{r^2} \frac{d}{dr} \left[ r \left( v + \frac{z}{r} \right)^2 \right] . \end{aligned}$$

The latter term equals

$$- \vec{\nabla} \cdot \left[ \frac{\vec{r}}{r^2} \left( v + \frac{z}{r} \right)^2 \right] ;$$

it is a divergence that integrates to a null result. Consequently,

$$E_2 = - \frac{1}{8\pi} \int (d\vec{r}) [\vec{\nabla} \left( v + \frac{z}{r} \right)]^2 = - \frac{1}{2} \int_0^\infty dr [r v]^2 ,$$

which then leads to the second integral in (108).

<sup>8</sup> J.P.Desclaux, At.Data Nucl.Data Tables 12, 311 (1973).

<sup>9</sup> E.Baker, Phys.Rev.36, 630 (1930).

<sup>10</sup> E. Hille, J. d'analyse Math. 23, 147 (1970) showed rigorously that the series (164) converges for small values of  $\sqrt{x}$ , certainly for  $\sqrt{x} < (108/3125)^{1/4} / \sqrt{B+2} = 0.227$ , possibly for somewhat larger values.

<sup>11</sup> A. Sommerfeld, Zschr. f. Phys. 78, 283 (1932).

<sup>12</sup> Some people call this the Coulson-March expansion [C.A.Coulson and N.H.March, Proc.Phys.Soc.London A 63, 367 (1950)].

<sup>13</sup> Hille (see Footnote 10) proved that the series (193) converges for sufficiently large values of  $x$ .

<sup>14</sup> Such a computer program was realized the first time by S.Kobayashi, T.Matsukuma, S.Nagai, and K.Umeda, J.Phys.Soc.Japan 10, 759 (1955). They truncated the expansion (193) after the  $k=17$  term. It is funny to observe that their coefficients  $c_1 \dots c_{10}$  are correct whereas  $c_{11} \dots c_{17}$  are wrong (with increasing error). This did, however, not affect their results as far as the values of  $B$  and  $\beta$ , given in the Abstract, are concerned. Also the decimales in their table of the TF function are correct.

- <sup>15</sup> The usefulness of this change of variables was first noticed by G.I.Plindov and I.K.Dmitrieva, Dokl.Akad.Nauk BSSR 19, 788 (1975).
- <sup>16</sup> A little bit more detail is reported in B.-G. Englert, Phys.Rev. A 33, 2146 (1986).
- <sup>17</sup> E.Fermi, Mem.Accad.d'Italia 1, 149 (1930). Fermi did not go beyond the first order. A systematic study of the expansion (316) was first presented by G.I.Plindov and I.K.Dmitrieva, Dokl.Akad.Nauk BSSR 21, 209 (1977).
- <sup>18</sup> G.I.Plindov and I.K.Dmitrieva, J.Phys. (Paris) 38, 1061 (1977).
- <sup>19</sup> B.-G.Englert, Zschr.f.Naturforschung 42a, 825 (1987).
- <sup>20</sup> This (physically rather obvious) statement has become known as the Lieb-Simon theorem after a formal proof was given by E.H.Lieb and B.Simon, Phys.Rev.Lett.31, 681 (1973). For more detail see the review by Lieb cited in Footnote 3 of Chapter One.
- <sup>21</sup> Cited in Footnote 2 of Chapter One.
- <sup>22</sup> Cited in Footnote 1 of Chapter One.
- <sup>23</sup> P. Hohenberg and W. Kohn, Phys.Rev. 136, B 864 (1964).
- <sup>24</sup> M. Levy and J.P. Perdew, Phys.Rev.A 32, 2010 (1985).
- <sup>25</sup> Cited in Footnote 2 of Chapter One.
- <sup>26</sup> Actually, (502), is a variant of Hartree's equations, inasmuch as the self energy is included and no averaging of  $V(\vec{r}')$  over its angular dependence is performed, which is a reasonable procedure in the situation of a spherically symmetric  $V_{\text{ext}}$ .
- <sup>27</sup> E.H. Lieb, Rev.Mod.Phys. 48, 553 (1976).
- <sup>28</sup> The corresponding  $\tilde{V}(r) = -(Z/r)\tilde{F}(x)$  is known as the Tietz potential [T.Tietz, Acta Phys.Hung.9, 73 (1958)].

Chapter Three.

<sup>1</sup> J.M.S. Scott, Philos. Mag. 43, 859 (1952).

<sup>2</sup> J. Schwinger, Phys. Rev. A 22, 1827 (1980).

<sup>3</sup> The additive constant that should, in principle, be included into the Coulomb potential,  $V(r) \approx -Z/r + \text{const.}$ , can be regarded as being part of  $\zeta_S$  and  $\zeta$ , respectively. Nothing is gained by displaying this constant explicitly, but the algebra is more transparent if one is not forced to keep track of this term, which for the present discussion is irrelevant anyhow.

<sup>4</sup> These (and all corresponding) polynomials in  $\langle y \rangle$  are closely related to the Bernoulli polynomials (Jakob Bernoulli, 1689). For example,

$$B_1(x + \frac{1}{2}) = x \quad ,$$

$$B_2(x + \frac{1}{2}) = x^2 - \frac{1}{12} \quad ,$$

and

$$B_3(x + \frac{1}{2}) = x^3 - \frac{1}{4}x \quad .$$

I owe this remark to Prof. G. Süßmann.

<sup>5</sup> Cited in Footnote 1 of Chapter One.

<sup>6</sup> In Lieb's review of 1981 (cited in Footnote 3 of Chapter One) there is the statement that "the Scott correction (...) is very plausible," but "has not yet been proved." This article was a contribution to a conference at Erice in June, 1980, which is a couple of months before Schwinger's paper appeared in print (November, 1980).

<sup>7</sup> B.-G. Englert and J. Schwinger, Phys. Rev. A 29, 2331 (1984). This paper has been the victim of absent-minded proofreading. Misprints that I am aware of are:

(1) in Eq. (24),  $v^2$  should read:  $\nabla^2$  ;

(2) the left-hand side of Eq. (40) should read:  $-\frac{1}{4\pi}\nabla^2 v$  ;

(3) in the first paragraph of the section "Scaling" read "scaling property" instead of "rescaling property;"

(4) in the second sentence of the same paragraph read "do two things for us" instead of "do the two things for us;"

- (5) Eq. (63) should read:  $B = 1.5880710\dots$  ;  
 (6) after Eq. (73) read "as  $Z$  scales to  $\lambda^{\beta-1} Z$ " instead of "as  $r$  scales to  $\lambda^{\beta-1} r$ ,"  
 (7) in the sum over  $j$  in Eq. (87) replace  $\zeta_i$  by  $\zeta_j$  ;  
 (8) in Eq. (88) replace " $\frac{b}{a} + Z^{4/3}$ " by " $\frac{b}{a} Z^{4/3}$ ,"  
 (9) the right-hand side of Eq. (102) should read:  $\frac{1}{3} Z^{-4/3}$  ;  
 (10) the last number in the first line of Table I should read: (-0.04).

<sup>8</sup> In Ref.7, there is the (wrong) statement that this [i.e., here Eq. (89), there Eq. (101)] is only approximately true — a misunderstanding caused by confusing the different meanings of  $Z$  in Eqs. (92) and (101).

<sup>9</sup> If  $a_1$  and  $a_2$  are, indeed, constants, the closed expression is

$$E_{\text{TFS}}(Z, N) = E_{\text{TF}}(Z, N - \frac{a_2}{6Z}) + \frac{1}{2} Z^2 - \frac{1}{4} a_1 Z \quad ,$$

which can be regarded as evidence in favor of the notion  $a_2 \geq 0$ .

- <sup>10</sup> This result has also been found, independently and almost simultaneously, by Bander whose argument is reminiscent of Scott's way of reasoning, and by Dmitrieva and Plindov who make an educated guess. The references are M. Bander, *Ann. Phys. (NY)* 144, 1 (1982); I.K. Dmitrieva and G.I. Plindov, *J. Phys. (Paris)* 43, 1599 (1982).
- <sup>11</sup> The HF predictions have been compiled on the basis of the orbital parameters given by S. Fraga, J. Karwowski, and K.M.S. Saxena, Handbook of Atomic Data (Elsevier, Amsterdam, 1976).
- <sup>12</sup> This is the main obstacle. The second-order TFS model has not been formulated as yet.
- <sup>13</sup> For more detail, consult Ref.7.

Chapter Four.

- <sup>1</sup> Consult, for instance, R.Finkelstein, Nonrelativistic Mechanics (Benjamin, Reading, Massachusetts, 1973), Chapter 3.
- <sup>2</sup> Of course, some such "wrong answers" are still better than others. For example, taking into account all contributions to  $\phi$  and  $T$  that are linear in  $V$ , improves the approximation significantly over the TF result of Eq.(19). In particular, the density at  $r=0$  turns out to be finite - but it does not have the correct value. For detail see R.K.Bhaduri, M.Brack, H.Gräf, and P.Schuck, J.Phys.Lett. (Paris) 41, L 347 (1980).
- <sup>3</sup> The derivation of (50) and (70) by R.K.Bhaduri, Phys.Rev.Lett. 39, 329 (1977) is, indeed, an expansion in powers of  $t$  (in  $\beta=it$  to be precise, but no matter). Bhaduri does not consider the  $\vec{s}$  dependence of  $\phi$ .
- <sup>4</sup> M.Durand, M.Brack, and P.Schuck, Zschr.f.Phys. A286, 381 (1978) arrive at Eqs.(45), (47), and (50) by "expanding in powers of  $\hbar$ " and in powers of  $\vec{s}$ .
- <sup>5</sup> E.Wigner, Phys.Rev. 40, 749 (1932); J.G.Kirkwood, Phys.Rev. 44, 31 (1933).
- <sup>6</sup> A standard reference is H.A.Antosiewicz, in Handbook of Mathematical Functions, edited by M.Abramowitz and I.Stegun (Dover, New York, 1972).
- <sup>7</sup> J.Schwinger, Phys.Rev. A 24, 2353 (1981).
- <sup>8</sup> B.-G.Englert and J.Schwinger, Phys.Rev. A 29, 2339 (1984).
- <sup>9</sup> C.F.von Weizsäcker, Zschr.f.Phys. 96, 431 (1935).
- <sup>10</sup> This statement is not entirely true, since a deficiency of von Weizsäcker's approach caused his result to be too large by a factor of nine. This, unfortunately, has induced people to consider that numerical factor as an adjustable parameter. (The "optimal" coefficient is then believed to be about 1/40 instead of 1/72.) I do not see the slightest justification for such a point of view. - To my knowledge the correct numerical multiple of  $(\vec{v}n)^2/n$  was first found

by A.Kompaneets and E.Pavlovskii, *Zh.Eksp.Teor.Fiz.* 31, 427 (1956) [*Sov.Phys. - JETP* 4, 328 (1957)], whose method is very different from the one used in the text. A procedure more closely related to ours is the one employed by D.Kirzhnits, *Zh.Eksp.Teor.Fiz.* 32, 115 (1957) [*Sov.Phys. - JETP* 5, 64 (1957)].

- <sup>11</sup> G.I.Plindov and I.K.Dmitrieva, *Phys.Lett.* 64A, 348 (1978), obtain a finite answer by introducing properly chosen cut-offs at small and large distances. They succeed in deriving (103) at the price of an electron cloud reminiscent of "an apricot without a stone," and of a wrong numerical coefficient for the Scott correction. Their procedure is therefore hardly convincing, although the correct  $Z^{5/3}$  term emerges.
- <sup>12</sup> Unfortunately, some (independent) earlier attempts of developing a quantum corrected description got either stuck or misled because the investigators did not succeed in evaluating the Airy integrals explicitly. See, in particular, R.Baltin, *Zschr.f.Naturforschung* A 27, 1176 (1972), and Ref.4.
- <sup>13</sup> Of some historical significance is the so-called "Amaldi correction" which aims at improving the original TF model by a rough guess of the electrostatic self-energy [E. Fermi and E. Amaldi, *Mem. Acc. Ital.* 6, 117 (1934)]. The arguments in favor of the Amaldi correction are not very strong in the first place (since certainly the Scott correction is more important), and they collapse totally as soon as exchange is included. It is, therefore, depressing to see people still handle models which contain both the exchange energy and the Amaldi correction.
- <sup>14</sup> Cited in Footnote 2 of Chapter One.
- <sup>15</sup> E. A. Milne, *Proc. Cambridge Philos. Soc.* 23, 794 (1927).
- <sup>16</sup> F. Rasetti, in: E. Fermi, Collected Papers (E. Amaldi et al., eds., Univ. of Chicago Press, 1962), p.277.
- <sup>17</sup> Cited in Footnote 9 of Chapter Two.
- <sup>18</sup> V. Bush and S.H. Caldwell, *Phys. Rev.* 38, 1898 (1931).

- <sup>19</sup> Cited in Footnote 14 of Chapter Two.
- <sup>20</sup> Cited in Footnote 1 of Chapter Three.
- <sup>21</sup> Cited in Footnote 1 of Chapter One.
- <sup>22</sup> Cited in Footnote 2 of Chapter Three.
- <sup>23</sup> See Footnote 7 of Chapter Three.
- <sup>24</sup> P.A.M. Dirac, Proc. Cambridge Philos. Soc. 26, 376 (1930).
- <sup>25</sup> Ref. 16, pp. 291-304.
- <sup>26</sup> H. Jensen, Zschr. f. Phys. 89, 713 (1934).
- <sup>27</sup> I.K. Dmitrieva and G.I. Plindov, cited in Footnote 10 of Chapter Three.
- <sup>28</sup> Cited in Footnote 11 of Chapter Three.
- <sup>29</sup> See Ref. 19 of Chapter Two.
- <sup>30</sup> Experimental ionization energies are tabulated by A.A. Radzig and B.M. Smirnov, Reference Data on Atoms, Molecules, and Ions (Springer, Berlin-Heidelberg, 1985) (Springer Series in Chemical Physics, Vol.31), for  $Z=1$  to  $Z=102$ , except for  $Z=85$  (astatine) and  $Z=87$  (francium) for which no spectroscopic data is reported. The stars for these elements in Fig.8 are the predictions of Ref. 19 of Chapter Two.
- <sup>31</sup> An illustration of this remark are the utterly wrong coefficients, corresponding to our Eq.(289), which are reported by S.H. Hill, P.J. Grout, and N.H. March, J. Phys. B 20, 11 (1987), in the appendix.
- <sup>32</sup> See Fig.20 in Gombás' textbook, cited in Footnote 1 of Chapter One.
- <sup>33</sup> I.K. Dmitrieva and G.I. Plindov, J. Phys. (Paris) 45, 85 (1984) give Padé approximants that interpolate between (302) and (303), and agree with these two limiting forms under the respective cir-

cumstances.

- <sup>34</sup> R.G. Parr, R.A. Donnelly, M. Levy, and W.E. Palke, *J. Chem. Phys.* 68, 3801 (1978).
- <sup>35</sup> W.E. Lamb, *Phys. Rev.* 60, 817 (1941).
- <sup>36</sup> The subscript  $m$  is non-standard; it is introduced only to exclude any confusion with  $\sigma = (7 + \sqrt{73})/2$ , defined in Eq. (2-309).
- <sup>37</sup> For  $Z \leq 86$  the HF numbers were compiled from the data given by C. Froese-Fischer, The Hartree-Fock Method for Atoms (Wiley, New York, 1977). For  $Z > 86$ , the (less precise) numbers of Ref. 11 of Chapter Three were used.
- <sup>38</sup> B.-G. Englert and J. Schwinger, *Phys. Rev. A* 26, 2322 (1982).
- <sup>39</sup> The potential  $\bar{V}$  in Eq. (13) of Ref. 38 equals  $U - U_{\text{ex}} + \zeta$ ; it is thus an electrostatic pseudo-potential. With this identification, (13) of Ref. 38 is equivalent to Eq. (342) in the text.
- <sup>40</sup> The external potential  $-Z/r$  has to be replaced by a sum over the Coulomb potentials of all the nuclei in the molecule; also the Scott term  $\frac{1}{2}Z^2$  becomes a sum over the contributions from individual nuclei. The level of sophistication in performing the CSBE in Eq. (331b) depends on the particular application. Further, if one is interested in the dependence of the energy on the parameters that specify the configuration of the nuclei, the electrostatic energy due to the Coulomb repulsion between the nuclei must be included. Effects of the finite nuclear masses are very small and certainly irrelevant at this level of accuracy.
- <sup>41</sup> As a matter of fact, what is discussed in the text is not the "usual argument" but a variant of it. The discussion is both simpler and more transparent this way.
- <sup>42</sup> Handbook of Chemistry and Physics (Chemical Rubber Co., Cleveland, Ohio, 1979/80).
- <sup>43</sup> F. Hoare and G. Brindley, *Proc. Roy. Soc. London* 159A, 395 (1937).

- <sup>44</sup> Sommerfeld's approximation to  $F(x)$ , that is  $F(x) \approx [1 + (12^{-2/3} x)^\gamma]^{-3/\gamma}$ , gives 8.71 for this integral. When inserted after undoing the two-fold partial integration, it produces 8.67. Both numbers are in satisfactory agreement with the actual value.
- <sup>45</sup> From Ref.11 of Chapter Three.
- <sup>46</sup> In Ref.24 of Chapter Two, Levy and Perdew try to put the blame for the discrepancy between experiment and the HF predictions entirely onto the experiments (or the experimentalists). This does not seem plausible to me. Also, relativistic corrections cannot account for differences this large.
- <sup>47</sup> B.-G. Englert and J. Schwinger, Phys. Rev. A29, 2353 (1984).
- <sup>48</sup> Another application is reported by A. Mañanes and E. Santos, Phys. Rev. B 34, 5874 (1986). Unfortunately, these authors confuse the potentials  $U$  and  $U_{es}$  (our denotation) with, luckily, no consequences as far as the conclusions of the paper are concerned. The appendix, however, and all related remarks in the text are erroneous.
- <sup>49</sup> This modified TF density (or its one-dimensional analog) has been derived prior to the publication of Ref.8 for the special situation of a linear potential, when (394) is the whole answer. I am aware of the following three papers: W. Kohn and L.J. Sham, Phys. Rev. 137, A1697 (1965); S.F. Timashev, Elektrokhemia 40, 730 (1979); H. Gräf, Nucl. Phys. A349, 349 (1980). All these authors squared the wave function in a linear potential [this is essentially an Airy function, see Eq.(143)] to arrive, finally, at (394) for that special potential. Our derivation is more general in not making such assumptions about  $V$ .
- <sup>50</sup> The subscript  $p$  is non-standard; it is introduced only to exclude any confusion with  $\alpha = 1.04018\dots$  of Eq.(2-313).
- <sup>51</sup> See Radzig and Smirnov, cited in Footnote 30.
- <sup>52</sup> The evaluation of the integral (140) and its  $y$ -derivative for  $x=0$  is a simple exercise in performing complex contour integrals. At worst, the results can be looked up in Ref.6.
- <sup>53</sup> The HF density is compiled from D.R. Hartree, Proc.Roy.Soc. London,

Ser. A 151, 96 (1935).

<sup>5 4</sup> L.L. DeRaad and J. Schwinger, Phys. Rev. A 25, 2399 (1982).

### Chapter Five.

<sup>1</sup> The first plot of this kind is contained in the paper by Dmitrieva and Plindov, cited in Footnote 10 to Chapter Three.

<sup>2</sup> To avoid a possible misunderstanding: it is not the numerical accuracy of HF numbers that is questioned here, but the physical reliability of the HF approximation.

<sup>3</sup> C.E. Moore, Atomic Energy Levels, Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 35 (U.S. GPO, Washington, D.C., 1970).

<sup>4</sup> J.P. Desclaux, cited in Footnote 8 to Chapter Two.

<sup>5</sup> J.M.S. Scott, cited in Footnote 1 to Chapter Three.

<sup>6</sup> H.A. Kramers, Zschr. f. Phys. 39, 836 (1926).

<sup>7</sup> R.E. Langer, Phys. Rev. 51, 669 (1937).

<sup>8</sup> N.H. March and J.S. Plaskett, Proc. R. Soc. London, Ser. A 235, 419 (1956) already noticed that the semiclassical sum contains the TF approximation in the continuum limit. However, their method is very different from the one discussed in this text, and they did not develop a systematic way of analyzing these quantum corrections.

<sup>9</sup> B.-G. Englert and J. Schwinger, Phys. Rev. A32, 26 (1985).

<sup>10</sup> The circular orbit is also the one which, for given angular momentum, has least energy.

<sup>11</sup> Presumably due to too crude an approximation for  $F(x)$ , Fermi reported 3.2 (instead of 3.916) for this integral in his classical paper on the systematics of the Periodic Table. The reference is:

E. Fermi, Rend. Lincei 7, 342 (1928).

- <sup>12</sup> B.-G. Englert and J. Schwinger, Phys. Rev. A 32, 36 (1985)
- <sup>13</sup> H. Hellmann, Acta Physicochim. URSS 4, 225 (1936), was the first to consider the  $\ell$ TF model. Since he used the original sum over  $\ell$ , not the Fourier formulation, Hellmann failed to recognize that one can split the energy into  $E_{TF}$  plus the quantum correction  $E_{qu}$ .
- <sup>14</sup> A simple counting of the respective points on a  $j, k$  lattice shows that this fraction equals  $[\arctan(v'_0) - \pi/4]/\pi = 0.098$ , a little bit less than ten percent.
- <sup>15</sup> The factor  $k-j$  is missing in Eqs.(107) and (108) of the original publication [B.-G. Englert and J. Schwinger, Phys. Rev. A 32, 47 (1986)]. Fortunately, this inadvertence did not cause any harm.
- <sup>16</sup> A standard reference is M. Abramowitz in the Handbook of Mathematical Functions, cited in Footnote 6 of Chapter Four.
- <sup>17</sup> Another way of plotting the Fresnel functions, and a particularly charming one, is presented in Fig.16 of F. Lösch, Tafeln höherer Funktionen/Tables of Higher Functions (7-th edition, Teubner, Stuttgart, 1966).
- <sup>18</sup> See the paper cited in Footnote 15.

## Chapter Six.

- <sup>1</sup> Density Functional Methods in Physics (Alcabideche/Portugal, 1983), edited by R.M. Dreizler and J. da Providência (Plenum Press, New York, 1985); Semiclassical Methods in Nuclear Physics (Grenoble/France, 1984), edited by R.W. Hasse, R. Arvieu, and P. Schuck, J. de Physique 45, Coll. C 6.
- <sup>2</sup> M.S. Vallarta and N. Rosen, Phys. Rev. 41, 708 (1932); H. Jensen, Zschr. f. Phys. 82, 794 (1933).
- <sup>3</sup> Footnote 3 of Chapter Three applies here as well.

<sup>4</sup> J. Schwinger, cited in Footnote 2 of Chapter Three.

<sup>5</sup> I.K. Dmitrieva and G.I. Plindov, cited in Footnote 10 of Chapter Three.

<sup>6</sup> From Ref.11 of Chapter Three.

<sup>7</sup> J.M.S. Scott, cited in Footnote 1 of Chapter Three.

<sup>8</sup> The number appearing here is

$$\begin{aligned}
 2.248 &= 4 \sum_{n=1}^{\infty} \frac{1}{n^5} - 19 \sum_{n=1}^{\infty} \frac{1}{n^4} + 4 \sum_{n=1}^{\infty} \sum_{m=1}^n \frac{1}{n^3} \frac{1}{m^2} + 12 \sum_{n=1}^{\infty} \sum_{m=1}^n \frac{1}{n^4} \frac{1}{m} \\
 &= 4 \times 1.036928 - 19 \times \frac{\pi^4}{90} + 4 \times 1.265738 + 12 \times 1.133479 \quad .
 \end{aligned}$$

<sup>9</sup> W. Kohn and L.J. Sham, Phys. Rev. 140, A1133 (1965)

<sup>10</sup> D.A. Kirzhnits and G.V. Shpatakovskaya, Zh. Eksp. Teor. Fiz. 62, 2082 (1972) [Sov. Phys. - JETP 35, 1088 (1972)] used methods related of those of Chapter Five to study shell effects in atomic densities. Their results are encouraging, but hardly satisfactory.

<sup>11</sup> E.P. Wigner, cited in Footnote 5 of Chapter Four. We do not include the factors of  $2\pi$  into the definition of the Wigner function. - A recent review of this subject is M. Hillary, R.F. O'Connell, M.O. Scully, and E.P. Wigner, Phys. Rep. 106, 121 (1984).