Condensed Matter Physics

PHY 5111

Dr Mohammad Abdur Rashid

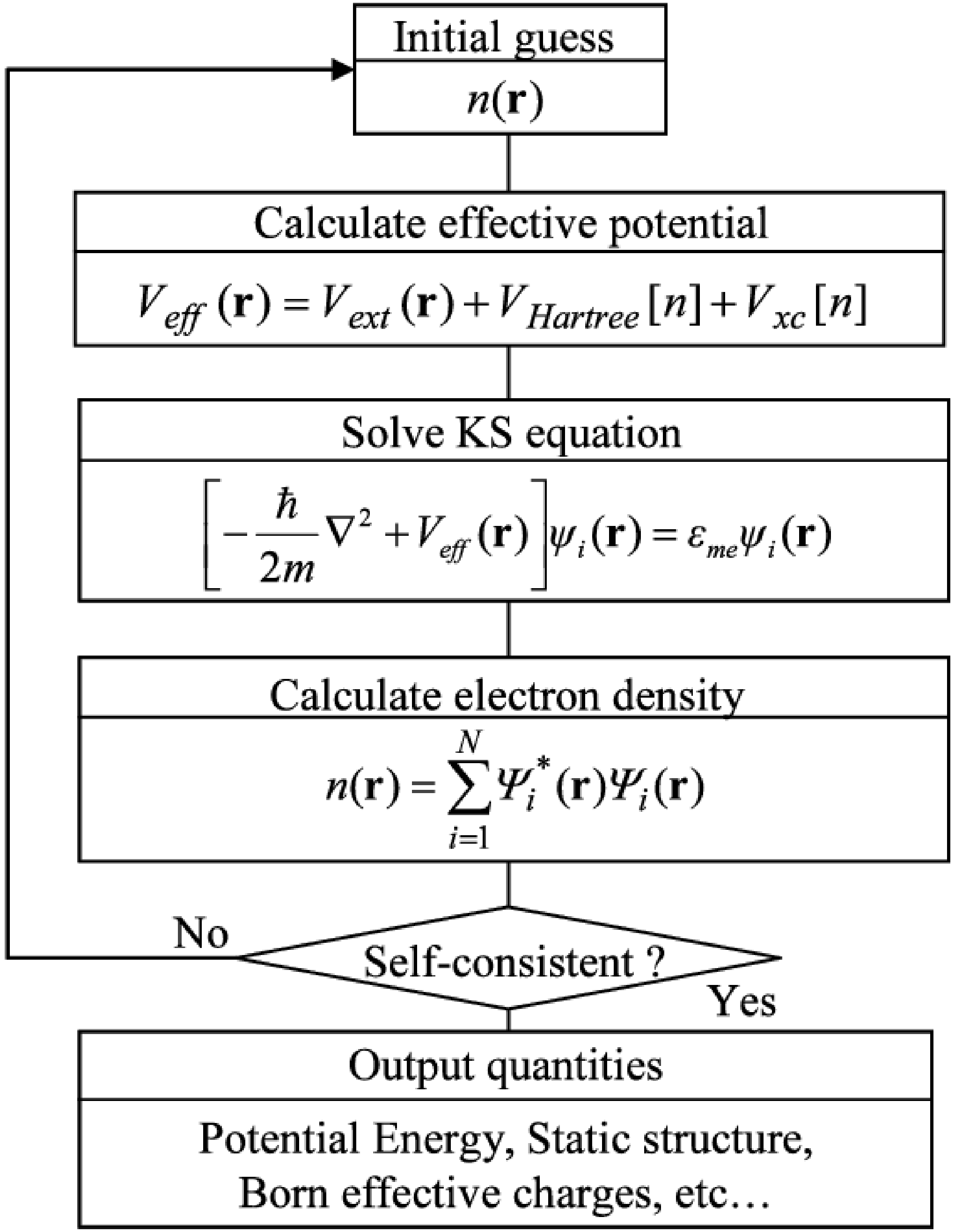
The kohn-Sham method: Elaboration

Density-Functional Theory of Atoms and Molecules
– Robert G. Parr and Weitao Yang

Chapter 8

Kohn-Sham method

$$v_{\text{eff}}(\mathbf{r}) = v(\mathbf{r}) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + v_{xc}(\mathbf{r})$$



Initial guess

$$n(\mathbf{r})$$

Calculate effective potential

$$V_{eff}(\mathbf{r}) = V_{ext}(\mathbf{r}) + V_{Hartree}[n] + V_{xc}[n]$$

Solve KS equation

$$\left[-\frac{\hbar}{2m}\nabla^2 + V_{eff}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \varepsilon_{me}\psi_i(\mathbf{r})$$

Calculate electron density

$$n(\mathbf{r}) = \sum_{i=1}^{N} \Psi_i^*(\mathbf{r})\Psi_i(\mathbf{r})$$

No

Self-consistent ?

Yes

Output quantities

Potential Energy, Static structure,
Born effective charges, etc…

Article to read

Perspective: Fifty years of density-functional theory in chemical physics

Cite as: J. Chem. Phys. **140**, 18A301 (2014); https://doi.org/10.1063/1.4869598
Submitted: 21 January 2014 . Accepted: 13 March 2014 . Published Online: 01 April 2014

Axel D. Becke

Local density approximation

$$E_{xc}^{\mathrm{LDA}}[\rho] = \int \rho(\mathbf{r})\varepsilon_{xc}(\rho)\, d\mathbf{r}$$

$$v_{xc}^{\mathrm{LDA}}(\mathbf{r}) = \frac{\delta E_{xc}^{\mathrm{LDA}}}{\delta\rho(\mathbf{r})} = \varepsilon_{xc}(\rho(\mathbf{r})) + \rho(\mathbf{r})\frac{\delta\varepsilon_{xc}(\rho)}{\delta\rho}$$

$$\boxed{\left[-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + v_{xc}^{\mathrm{LDA}}(\mathbf{r})\right]\psi_i = \varepsilon_i\psi_i.}$$

Local density approximation

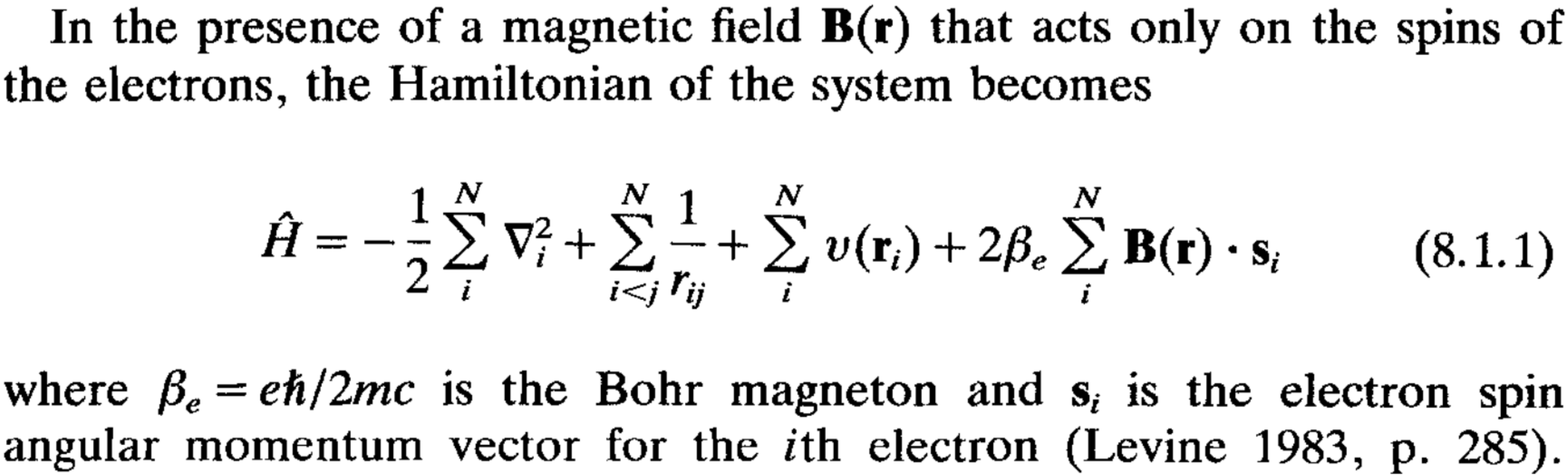
$$\varepsilon_{xc}(\rho) = \varepsilon_x(\rho) + \varepsilon_c(\rho)$$

$$\varepsilon_x(\rho) = -C_x \rho(\mathbf{r})^{1/3}, \qquad C_x = \frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}$$

$$\varepsilon_c(r_s) = \frac{A}{2}\left\{\ln\frac{x}{X(x)} + \frac{2b}{Q}\tan^{-1}\frac{Q}{2x+b} - \frac{bx_0}{X(x_0)}\left[\ln\frac{(x-x_0)^2}{X(x)} + \frac{2(b+2x_0)}{Q}\tan^{-1}\frac{Q}{2x+b}\right]\right\} \quad \text{(E.27)}$$

where $x = r_s^{1/2}$, $X(x) = x^2 + bx + c$, and $Q = (4c - b^2)^{1/2}$. For $\varepsilon_c^0(r_s)$, $A = 0.0621814$, $x_0 = -0.409286$, $b = 13.0720$, and $c = 42.7198$; for $\varepsilon_c^1(r_s)$, $A = \frac{1}{2}(0.0621814)$, $x_0 = -0.743294$, $b = 20.1231$, and $c = 101.578$. These formulas are generally accepted as the most accurate available for the uniform-gas correlation energy per particle.

Spin-density functional theory



In the presence of a magnetic field $\mathbf{B}(\mathbf{r})$ that acts only on the spins of the electrons, the Hamiltonian of the system becomes

$$\hat{H} = -\frac{1}{2}\sum_{i}^{N}\nabla_i^2 + \sum_{i<j}^{N}\frac{1}{r_{ij}} + \sum_{i}^{N} v(\mathbf{r}_i) + 2\beta_e \sum_{i}^{N} \mathbf{B}(\mathbf{r})\cdot\mathbf{s}_i \qquad (8.1.1)$$

where $\beta_e = e\hbar/2mc$ is the Bohr magneton and $\mathbf{s}_i$ is the electron spin angular momentum vector for the ith electron (Levine 1983, p. 285).

Spin-density functional theory

$$\hat{V} = \sum_{i}^{N} v(\mathbf{r}_i) + 2\beta_e \sum_{i}^{N} \mathbf{B}(\mathbf{r}_i) \cdot \mathbf{s}_i$$

$$= \int v(\mathbf{r})\hat{\rho}(\mathbf{r})\, d\mathbf{r} - \int \mathbf{B}(\mathbf{r}) \cdot \hat{\mathbf{m}}(\mathbf{r})\, d\mathbf{r}$$

$$\hat{\mathbf{m}}(\mathbf{r}) = -2\beta_e \sum_{i}^{N} \mathbf{s}_i\, \delta(\mathbf{r} - \mathbf{r}_i)$$

$$\hat{\rho}(\mathbf{r}) = \sum_{i}^{N} \delta(\mathbf{r} - \mathbf{r}_i)$$

$$\langle \Psi | \hat{V} | \Psi \rangle = \int v(\mathbf{r})\rho(\mathbf{r})\, d\mathbf{r} - \int \mathbf{B}(\mathbf{r}) \cdot \mathbf{m}(\mathbf{r})\, d\mathbf{r}$$

$$\rho(\mathbf{r}) = \langle \Psi | \hat{\rho}(\mathbf{r}) | \Psi \rangle$$

$$\mathbf{m}(\mathbf{r}) = \langle \Psi | \hat{\mathbf{m}}(\mathbf{r}) | \Psi \rangle$$

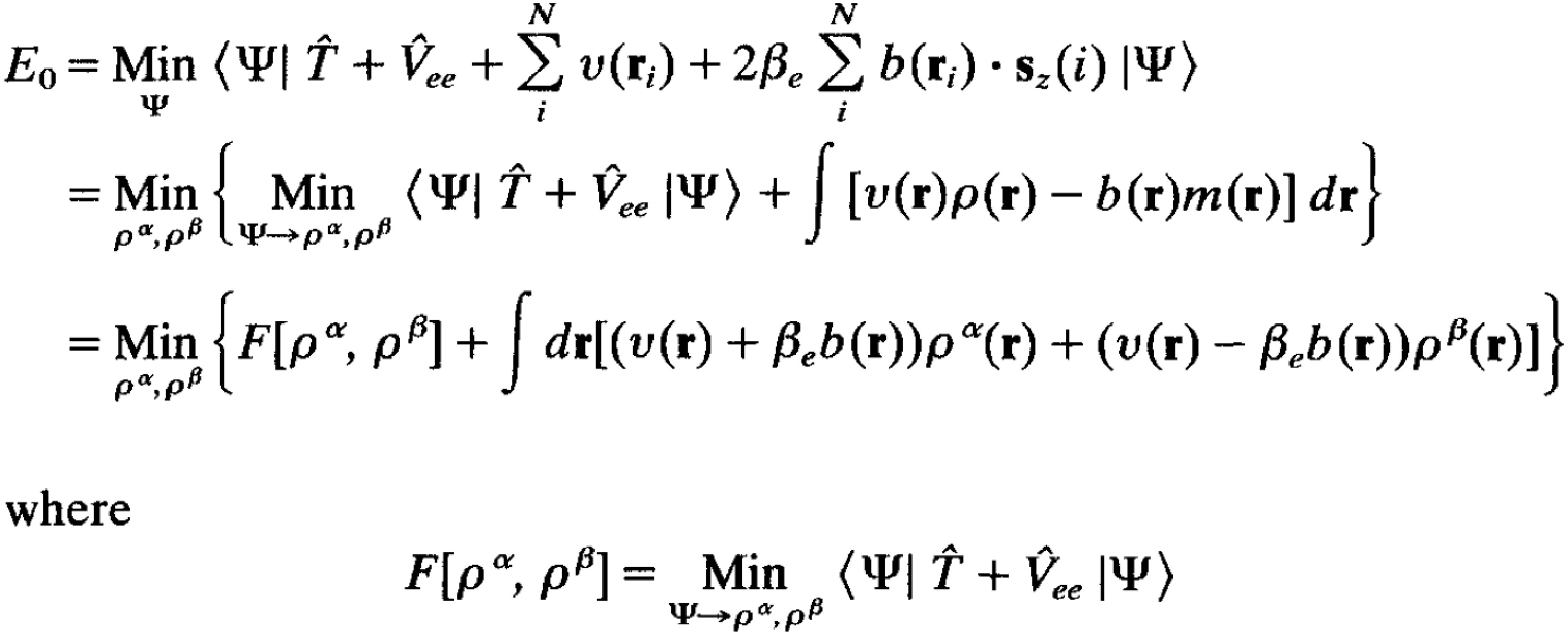
$$\langle \Psi | \hat{V} | \Psi \rangle = \int v(\mathbf{r})\rho(\mathbf{r})\, d\mathbf{r} - \int b(\mathbf{r}) m(\mathbf{r})\, d\mathbf{r}$$

We shall discuss only the simple case of z-direction $b(\mathbf{r})$

Spin-density functional theory

$$
\begin{aligned}
m(\mathbf{r}) &= -2\beta_e \langle \Psi | \sum_{i}^{N} s_z(i)\, \delta(\mathbf{r}-\mathbf{r}_i)\, |\Psi\rangle \\
&= -2\beta_e \int s_z\, \delta(\mathbf{r}-\mathbf{r}')\gamma_1(\mathbf{x}', \mathbf{x}')\, d\mathbf{x}' \\
&= -2\beta_e \sum_{s=\alpha,\beta} s_z \gamma_1(\mathbf{r}s, \mathbf{r}s) \\
&= -2\beta_e[\tfrac{1}{2}\gamma_1(\mathbf{r}\alpha, \mathbf{r}\alpha) + (-\tfrac{1}{2})\gamma_1(\mathbf{r}\beta, \mathbf{r}\beta)] \\
&= \beta_e[\rho^{\beta}(\mathbf{r}) - \rho^{\alpha}(\mathbf{r})]
\end{aligned}
$$

Spin-density functional theory



$$E_0 = \underset{\Psi}{\mathrm{Min}} \langle \Psi | \hat{T} + \hat{V}_{ee} + \sum_i^N v(\mathbf{r}_i) + 2\beta_e \sum_i^N b(\mathbf{r}_i) \cdot \mathbf{s}_z(i) | \Psi \rangle$$

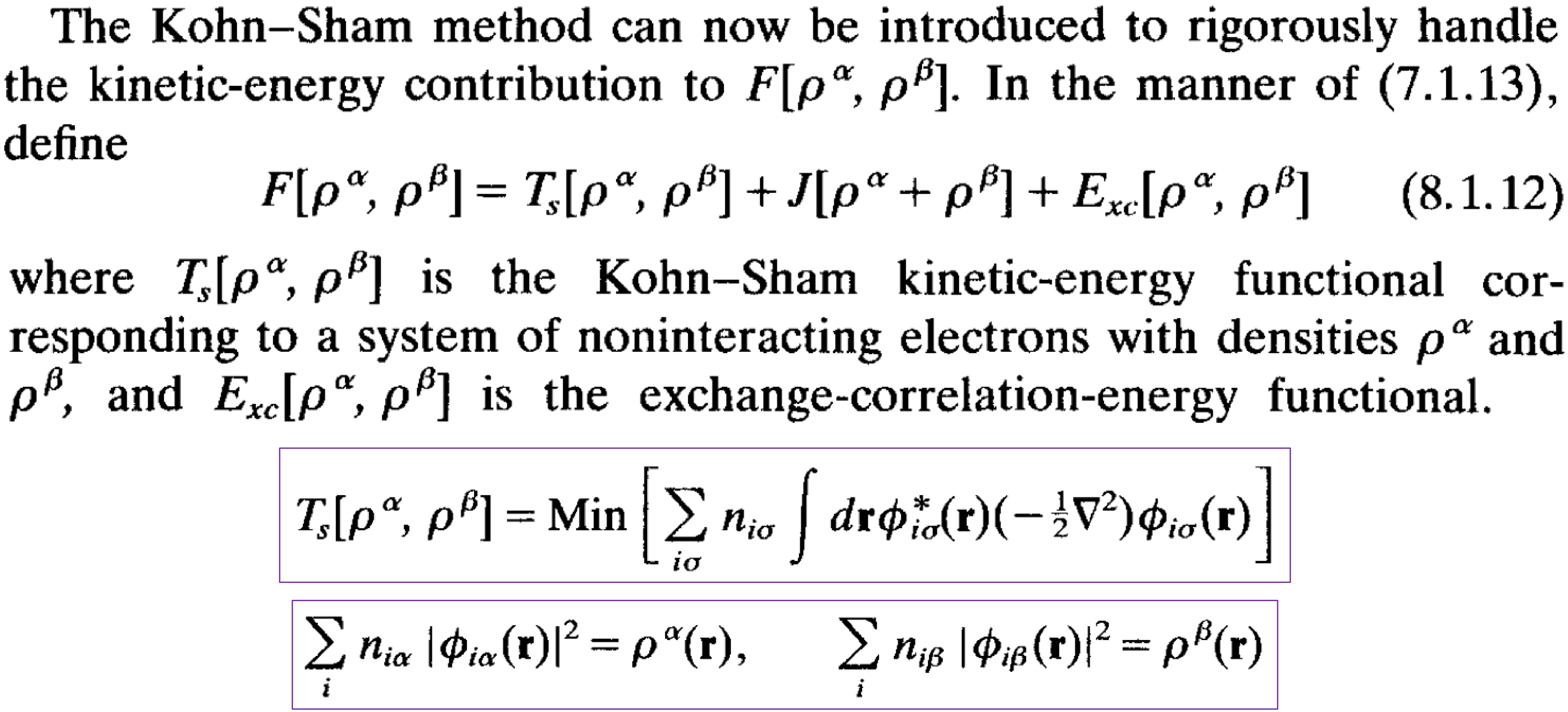
$$= \underset{\rho^\alpha, \rho^\beta}{\mathrm{Min}} \left\{ \underset{\Psi \to \rho^\alpha, \rho^\beta}{\mathrm{Min}} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle + \int [v(\mathbf{r})\rho(\mathbf{r}) - b(\mathbf{r}) m(\mathbf{r})] \, d\mathbf{r} \right\}$$

$$= \underset{\rho^\alpha, \rho^\beta}{\mathrm{Min}} \left\{ F[\rho^\alpha, \rho^\beta] + \int d\mathbf{r} [(v(\mathbf{r}) + \beta_e b(\mathbf{r}))\rho^\alpha(\mathbf{r}) + (v(\mathbf{r}) - \beta_e b(\mathbf{r}))\rho^\beta(\mathbf{r})] \right\}$$

where

$$F[\rho^\alpha, \rho^\beta] = \underset{\Psi \to \rho^\alpha, \rho^\beta}{\mathrm{Min}} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle$$

Spin-density functional theory



The Kohn–Sham method can now be introduced to rigorously handle the kinetic-energy contribution to $F[\rho^\alpha, \rho^\beta]$. In the manner of (7.1.13), define

$$F[\rho^\alpha, \rho^\beta] = T_s[\rho^\alpha, \rho^\beta] + J[\rho^\alpha + \rho^\beta] + E_{xc}[\rho^\alpha, \rho^\beta] \qquad (8.1.12)$$

where $T_s[\rho^\alpha, \rho^\beta]$ is the Kohn–Sham kinetic-energy functional corresponding to a system of noninteracting electrons with densities ρ^α and ρ^β, and $E_{xc}[\rho^\alpha, \rho^\beta]$ is the exchange-correlation-energy functional.

$$\boxed{T_s[\rho^\alpha, \rho^\beta] = \mathrm{Min}\left[\sum_{i\sigma} n_{i\sigma} \int d\mathbf{r}\,\phi_{i\sigma}^*(\mathbf{r})\left(-\tfrac{1}{2}\nabla^2\right)\phi_{i\sigma}(\mathbf{r})\right]}$$

$$\boxed{\sum_i n_{i\alpha}\,|\phi_{i\alpha}(\mathbf{r})|^2 = \rho^\alpha(\mathbf{r}), \qquad \sum_i n_{i\beta}\,|\phi_{i\beta}(\mathbf{r})|^2 = \rho^\beta(\mathbf{r})}$$

Spin-density functional theory

$$\boxed{T_s[\rho^\alpha, \rho^\beta] = \sum_{i\sigma} n_{i\sigma} \int d\mathbf{r}\phi^*_{i\sigma}(\mathbf{r})(-\tfrac{1}{2}\nabla^2)\phi_{i\sigma}(\mathbf{r})}$$

$$E[\rho^\alpha, \rho^\beta] = \sum_{i\sigma} n_{i\sigma} \int d\mathbf{r}\phi^*_{i\sigma}(\mathbf{r})(-\tfrac{1}{2}\nabla^2)\phi_{i\sigma}(\mathbf{r}) + J[\rho^\alpha + \rho^\beta] + E_{xc}[\rho^\alpha, \rho^\beta]$$

$$+ \int d\mathbf{r}[(v(\mathbf{r}) + \beta_e b(\mathbf{r}))\rho^\alpha(\mathbf{r}) + (v(\mathbf{r}) - \beta_e b(\mathbf{r})\rho^\beta(\mathbf{r}))] \qquad (8.1.16)$$

The variational search for the minimum of $E[\rho^\alpha, \rho^\beta]$ can then be carried out through orbitals, subject to normalization constraints:

$$\int \phi_{i\sigma}(\mathbf{r})\phi_{i\sigma}(\mathbf{r})\, d\mathbf{r} = 1 \qquad (8.1.17)$$

Spin-density functional theory

The resulting Kohn–Sham equations are

$$\hat{h}^{\alpha}_{\text{eff}}\phi_{i\alpha}(\mathbf{r}) = [-\tfrac{1}{2}\nabla^2 + v^{\alpha}_{\text{eff}}(\mathbf{r})]\phi_{i\alpha}(\mathbf{r})$$

$$= \frac{\varepsilon'_{i\alpha}}{n_{i\alpha}}\phi_{i\alpha}(\mathbf{r}) = \varepsilon_{i\alpha}\phi_{i\alpha}(\mathbf{r}), \qquad i = 1, 2, \ldots, N^{\alpha}$$

$$\hat{h}^{\beta}_{\text{eff}}\phi_{j\beta}(\mathbf{r}) = [-\tfrac{1}{2}\nabla^2 + v^{\beta}_{\text{eff}}(\mathbf{r})]\phi_{j\beta}(\mathbf{r})$$

$$= \frac{\varepsilon'_{j\beta}}{n_{j\beta}}\phi_{j\beta}(\mathbf{r}) = \varepsilon_{j\beta}\phi_{j\beta}(\mathbf{r}), \qquad j = 1, 2, \ldots, N^{\beta}$$

$$N^{\alpha} = \int d\mathbf{r}\,\rho^{\alpha}(\mathbf{r}), \qquad N^{\beta} = \int d\mathbf{r}\,\rho^{\beta}(\mathbf{r})$$

$$N = N^{\alpha} + N^{\beta}$$

Spin-density functional theory

where the spin-dependent effective potentials are

$$v_{\text{eff}}^{\alpha} = v(\mathbf{r}) + \beta_e b(\mathbf{r}) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \frac{\delta E_{xc}[\rho^{\alpha}, \rho^{\beta}]}{\delta \rho^{\alpha}(\mathbf{r})}$$

$$v_{\text{eff}}^{\beta} = v(\mathbf{r}) - \beta_e b(\mathbf{r}) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \frac{\delta E_{xc}[\rho^{\alpha}, \rho^{\beta}]}{\delta \rho^{\beta}(\mathbf{r})}$$

$$\boxed{N^{\alpha} = \int d\mathbf{r}\, \rho^{\alpha}(\mathbf{r}), \qquad N^{\beta} = \int d\mathbf{r}\, \rho^{\beta}(\mathbf{r})} \qquad \boxed{N = N^{\alpha} + N^{\beta}}$$

Spin-density functional theory

$$\boxed{T_s[\rho^\alpha, \rho^\beta] = \sum_{i\sigma} n_{i\sigma} \int d\mathbf{r}\phi^*_{i\sigma}(\mathbf{r})(-\tfrac{1}{2}\nabla^2)\phi_{i\sigma}(\mathbf{r})}$$

$$T_s[\rho^\alpha, \rho^\beta] = T_s[\rho^\alpha, 0] + T_s[0, \rho^\beta]$$

$$T_s[\rho^\alpha, 0] = \sum_{i\alpha} n_{i\alpha} \int d\mathbf{r}\, \phi^*_{i\alpha}(\mathbf{r})(-\tfrac{1}{2}\nabla^2)\phi_{i\alpha}(\mathbf{r})$$

$$\boxed{\rho^\alpha(\mathbf{r}) = \rho^\beta(\mathbf{r}) = \tfrac{1}{2}\rho(\mathbf{r})}$$

Spin-density functional theory

$$\begin{aligned} T_s[\tfrac{1}{2}\rho, \tfrac{1}{2}\rho] &= T_s[\tfrac{1}{2}\rho, 0] + T_s[0, \tfrac{1}{2}\rho] \\ &= 2T_s[\tfrac{1}{2}\rho, 0] \end{aligned}$$

$$\boxed{\rho^{\alpha}(\mathbf{r}) = \rho^{\beta}(\mathbf{r}) = \tfrac{1}{2}\rho(\mathbf{r})}$$

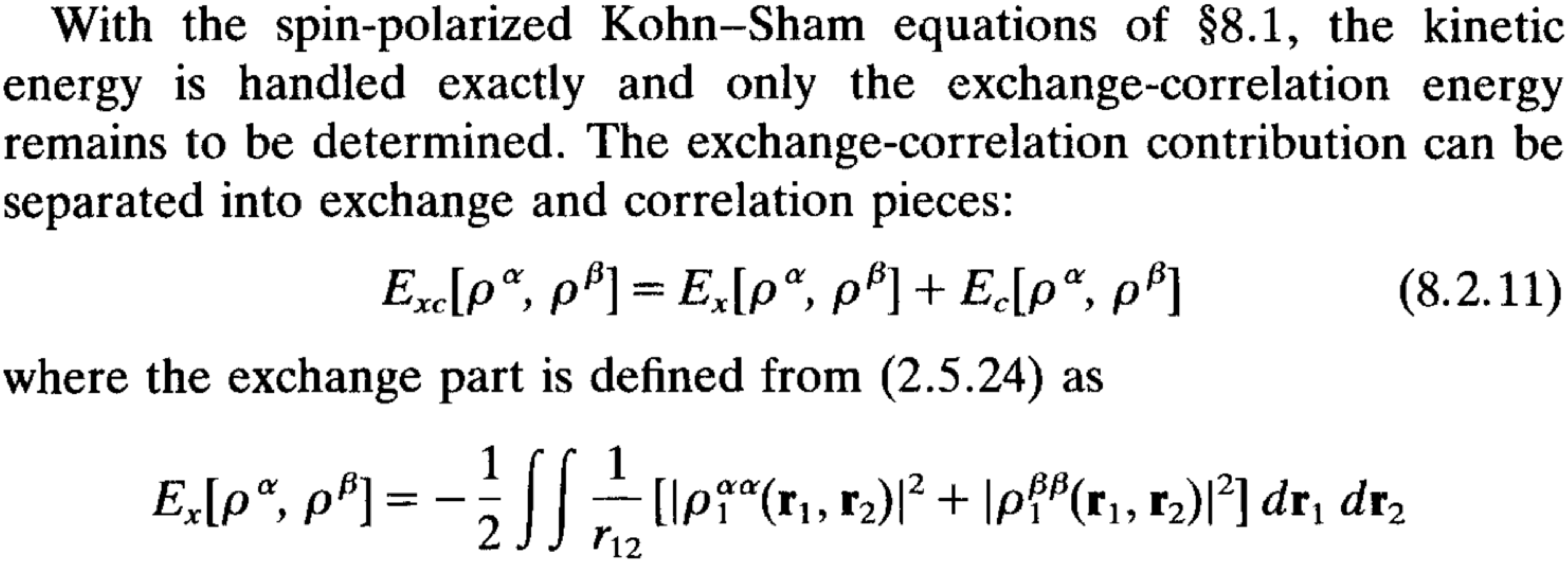
$$T_s[\tfrac{1}{2}\rho, 0] = T_s[0, \tfrac{1}{2}\rho]$$

$$\boxed{T_s[\rho^{\alpha}, \rho^{\beta}] = T_s[\rho^{\alpha}, 0] + T_s[0, \rho^{\beta}]}$$

$$T_s^0[\rho] = T_s[\tfrac{1}{2}\rho, \tfrac{1}{2}\rho]$$

$$\boxed{T_s[\rho^{\alpha}, \rho^{\beta}] = \tfrac{1}{2}T_s^0[2\rho^{\alpha}] + \tfrac{1}{2}T_s^0[2\rho^{\beta}]}$$

Spin-density functionals and the local spin-density approximations



With the spin-polarized Kohn–Sham equations of §8.1, the kinetic energy is handled exactly and only the exchange-correlation energy remains to be determined. The exchange-correlation contribution can be separated into exchange and correlation pieces:

$$E_{xc}[\rho^{\alpha}, \rho^{\beta}] = E_x[\rho^{\alpha}, \rho^{\beta}] + E_c[\rho^{\alpha}, \rho^{\beta}] \qquad (8.2.11)$$

where the exchange part is defined from (2.5.24) as

$$E_x[\rho^{\alpha}, \rho^{\beta}] = -\frac{1}{2}\iint \frac{1}{r_{12}}\left[|\rho_1^{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\rho_1^{\beta\beta}(\mathbf{r}_1, \mathbf{r}_2)|^2\right] d\mathbf{r}_1\, d\mathbf{r}_2$$

Spin-density functionals and the local spin-density approximations

$$E_x[\rho^{\alpha}, \rho^{\beta}] = -\frac{1}{2}\iint \frac{1}{r_{12}}\left[|\rho_1^{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\rho_1^{\beta\beta}(\mathbf{r}_1, \mathbf{r}_2)|^2\right] d\mathbf{r}_1\, d\mathbf{r}_2$$

$$\rho_1^{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}_2) = \sum_i n_{i\alpha}\phi_{i\alpha}(\mathbf{r}_1)\phi_{i\alpha}^*(\mathbf{r}_2)$$

$$\rho_1^{\beta\beta}(\mathbf{r}_1, \mathbf{r}_2) = \sum_i n_{i\beta}\phi_{i\beta}(\mathbf{r}_1)\phi_{i\beta}^*(\mathbf{r}_2)$$

Spin-density functionals and the local spin-density approximations

$$
\begin{aligned}
E_x[\rho^\alpha, \rho^\beta] &= \tfrac{1}{2}E_x[\rho^\alpha, \rho^\alpha] + \tfrac{1}{2}E_x[\rho^\beta, \rho^\beta] \\
&= \tfrac{1}{2}E_x^0[2\rho^\alpha] + \tfrac{1}{2}E_x^0[2\rho^\beta]
\end{aligned}
$$

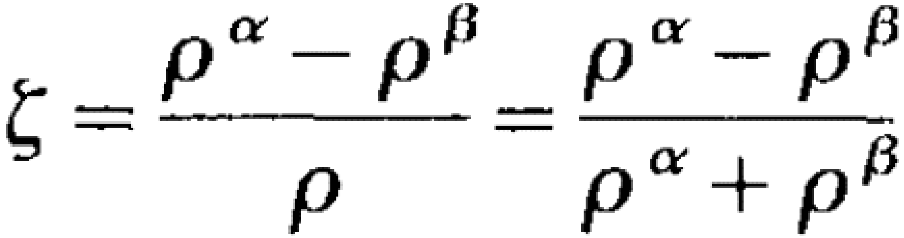
$$E_x^0[\rho] = E_x[\tfrac{1}{2}\rho, \tfrac{1}{2}\rho]$$

$$\boxed{E_x^{\mathrm{LSD}}[\rho^\alpha, \rho^\beta] = 2^{1/3}C_x \int [(\rho^\alpha)^{4/3} + (\rho^\beta)^{4/3}]\, d\mathbf{r}}$$

Local spin-density approximation (LSD)

Spin-density functionals and the local spin-density approximations

Define the spin polarization parameter ζ by



$$\zeta \equiv \frac{\rho^{\alpha} - \rho^{\beta}}{\rho} = \frac{\rho^{\alpha} - \rho^{\beta}}{\rho^{\alpha} + \rho^{\beta}}$$

Spin-density functionals and the local spin-density approximations

Then $\rho^{\alpha} = \frac{1}{2}(1+\zeta)\rho$, $\rho^{\beta} = \frac{1}{2}(1-\zeta)\rho$, and the LSD exchange energy becomes

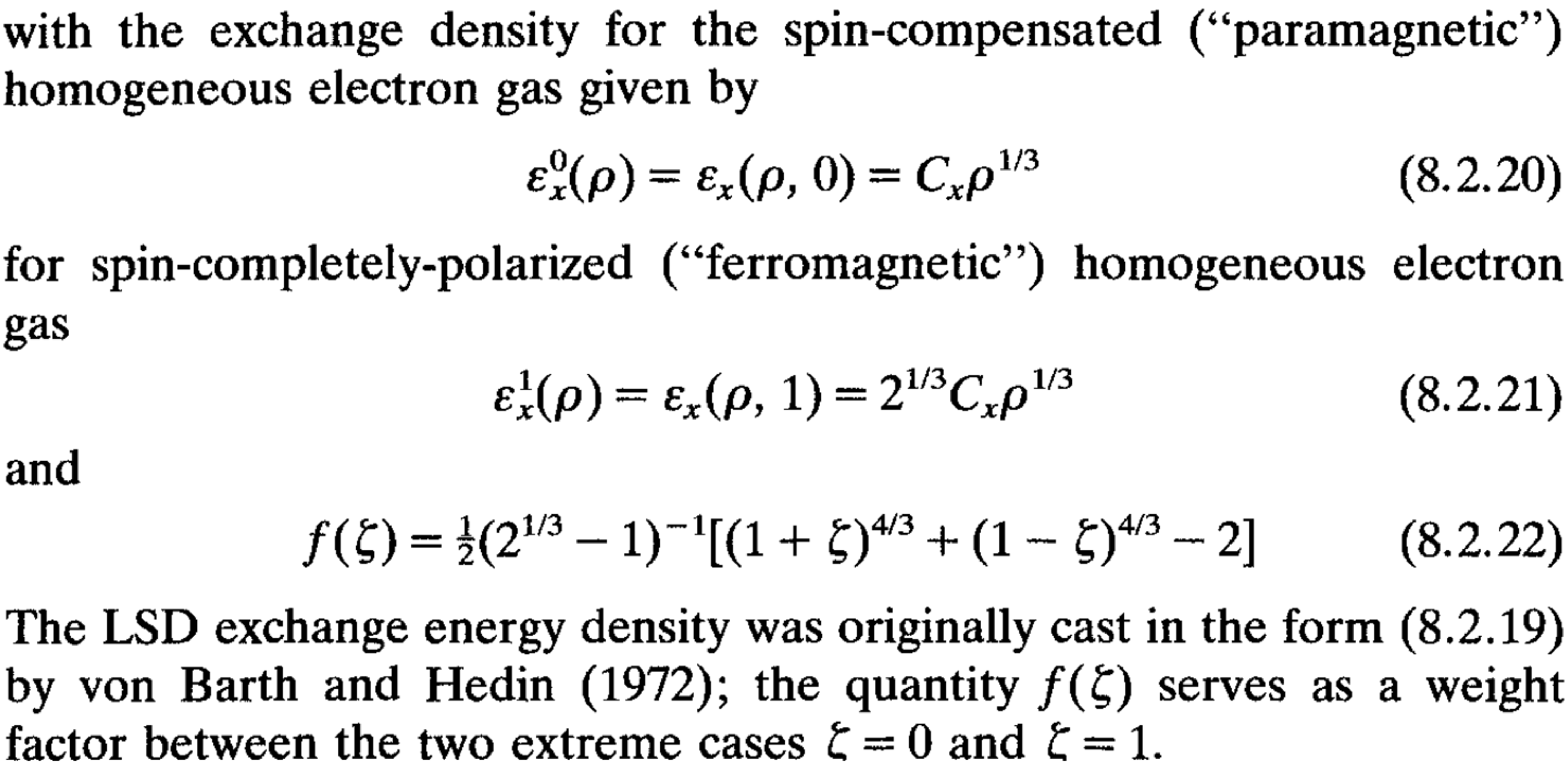
$$E_x^{\mathrm{LSD}}[\rho^{\alpha}, \rho^{\beta}] = \frac{1}{2}C_x \int \rho^{4/3}[(1+\zeta)^{4/3} + (1-\zeta)^{4/3}]\, d\mathbf{r}$$

$$= \int \rho\varepsilon_x(\rho, \zeta)\, d\mathbf{r} \qquad (8.2.18)$$

where

$$\varepsilon_x(\rho, \zeta) = \varepsilon_x^0(\rho) + [\varepsilon_x^1(\rho) - \varepsilon_x^0(\rho)]f(\zeta) \qquad (8.2.19)$$

Spin-density functionals and the local spin-density approximations



with the exchange density for the spin-compensated (“paramagnetic”) homogeneous electron gas given by

$$\varepsilon_x^0(\rho) = \varepsilon_x(\rho, 0) = C_x\rho^{1/3} \tag{8.2.20}$$

for spin-completely-polarized (“ferromagnetic”) homogeneous electron gas

$$\varepsilon_x^1(\rho) = \varepsilon_x(\rho, 1) = 2^{1/3}C_x\rho^{1/3} \tag{8.2.21}$$

and

$$f(\zeta) = \tfrac{1}{2}(2^{1/3} - 1)^{-1}[(1 + \zeta)^{4/3} + (1 - \zeta)^{4/3} - 2] \tag{8.2.22}$$

The LSD exchange energy density was originally cast in the form (8.2.19) by von Barth and Hedin (1972); the quantity $f(\zeta)$ serves as a weight factor between the two extreme cases $\zeta = 0$ and $\zeta = 1$.

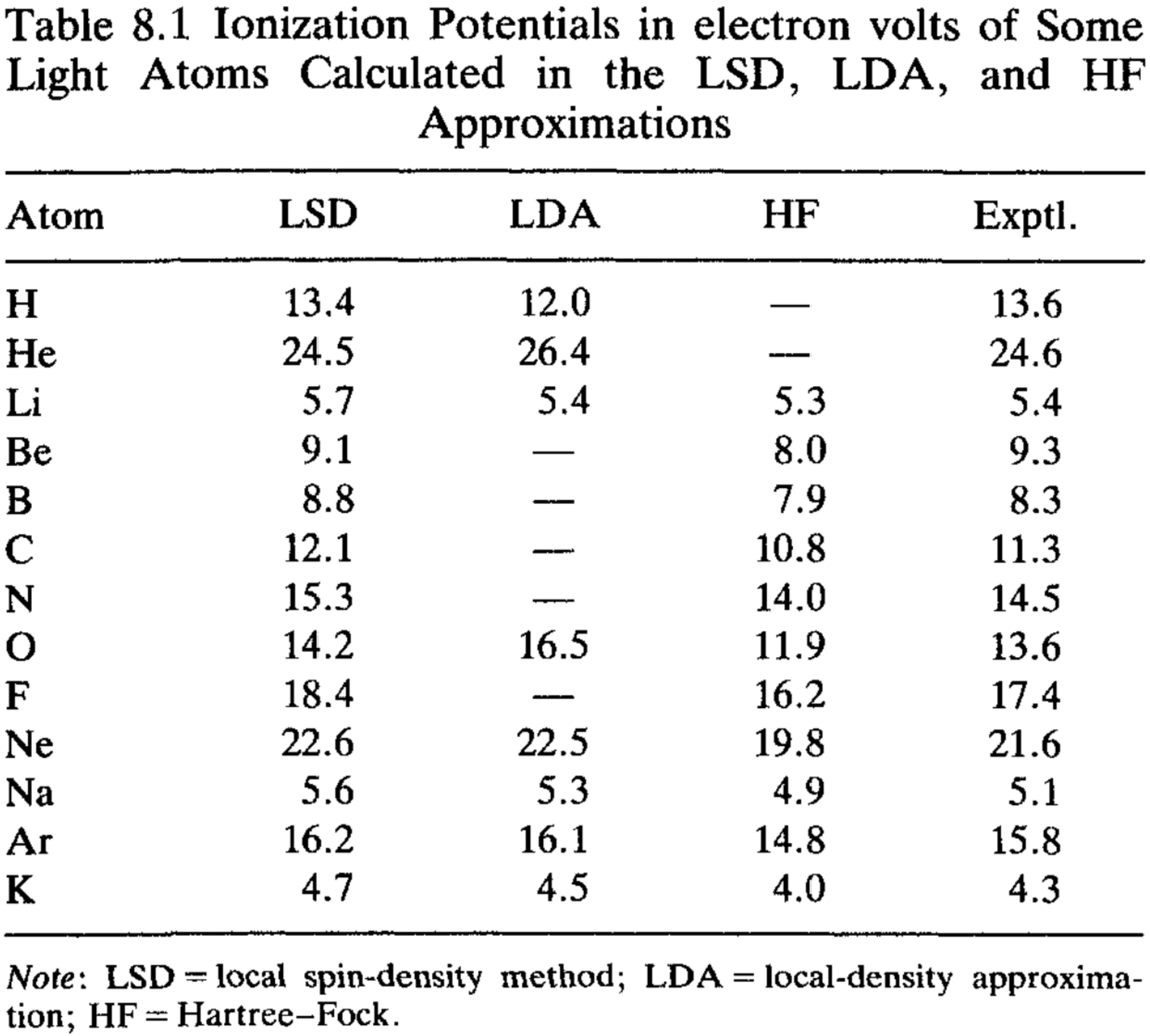


Table 8.1 Ionization Potentials in electron volts of Some Light Atoms Calculated in the LSD, LDA, and HF Approximations

Atom	LSD	LDA	HF	Exptl.
H	13.4	12.0	—	13.6
He	24.5	26.4	—	24.6
Li	5.7	5.4	5.3	5.4
Be	9.1	—	8.0	9.3
B	8.8	—	7.9	8.3
C	12.1	—	10.8	11.3
N	15.3	—	14.0	14.5
O	14.2	16.5	11.9	13.6
F	18.4	—	16.2	17.4
Ne	22.6	22.5	19.8	21.6
Na	5.6	5.3	4.9	5.1
Ar	16.2	16.1	14.8	15.8
K	4.7	4.5	4.0	4.3

Note: LSD = local spin-density method; LDA = local-density approximation; HF = Hartree–Fock.

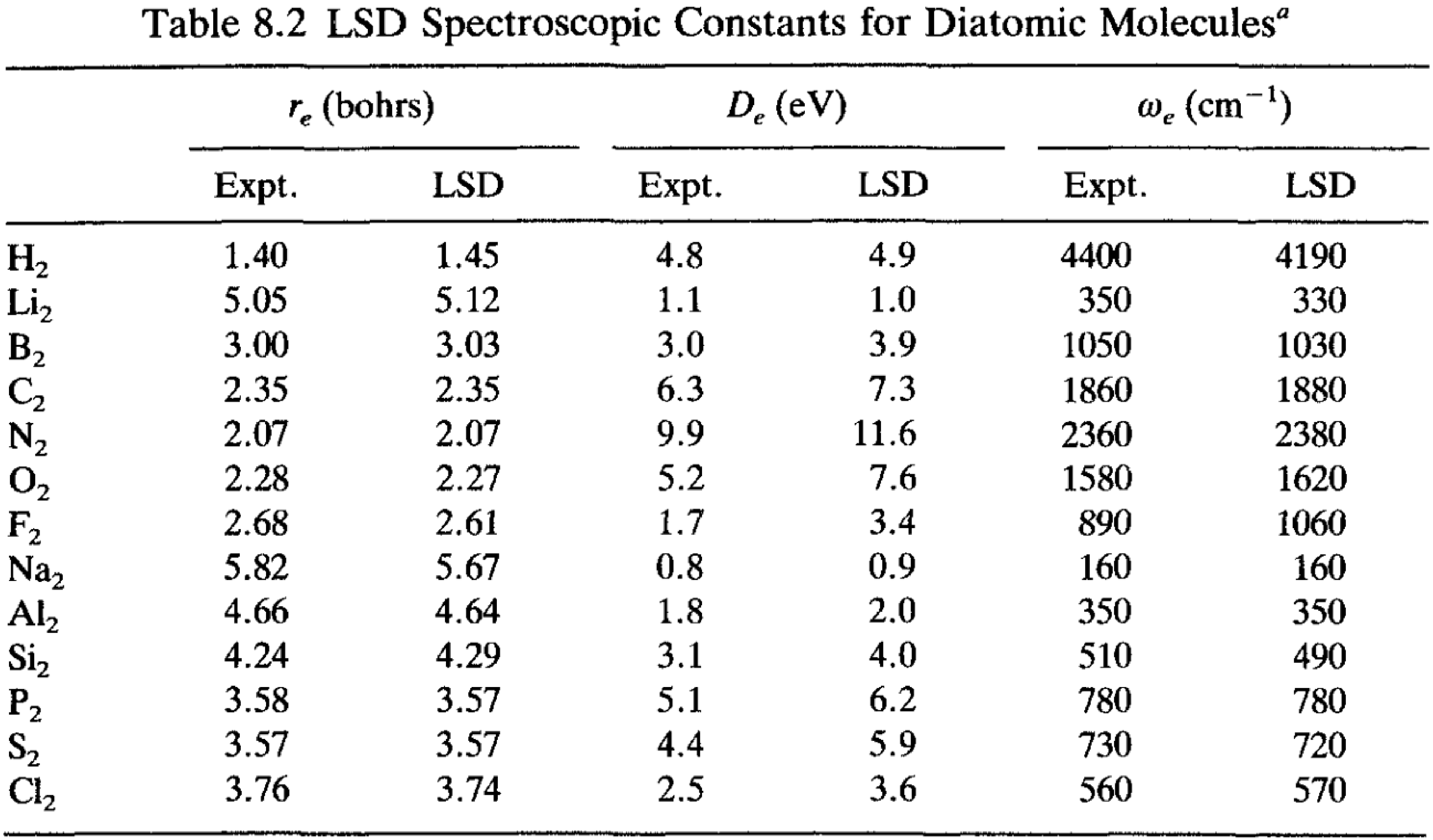
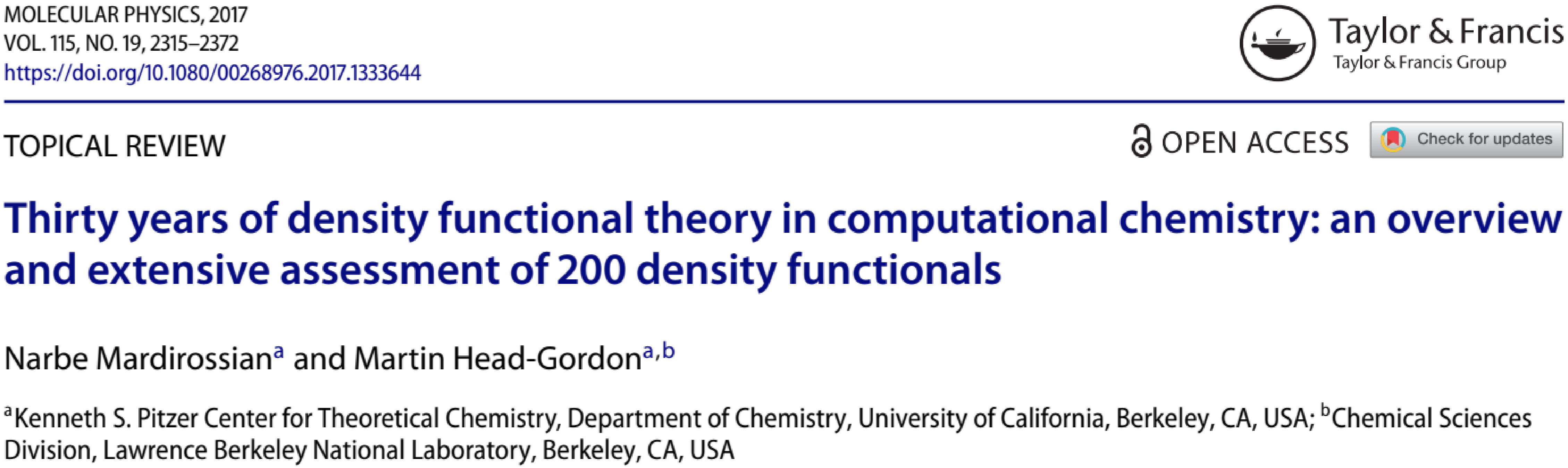


Table 8.2 LSD Spectroscopic Constants for Diatomic Molecules[a]

	r_e (bohrs)		D_e (eV)		ω_e (cm^{-1})	
	Expt.	LSD	Expt.	LSD	Expt.	LSD
H_2	1.40	1.45	4.8	4.9	4400	4190
Li_2	5.05	5.12	1.1	1.0	350	330
B_2	3.00	3.03	3.0	3.9	1050	1030
C_2	2.35	2.35	6.3	7.3	1860	1880
N_2	2.07	2.07	9.9	11.6	2360	2380
O_2	2.28	2.27	5.2	7.6	1580	1620
F_2	2.68	2.61	1.7	3.4	890	1060
Na_2	5.82	5.67	0.8	0.9	160	160
Al_2	4.66	4.64	1.8	2.0	350	350
Si_2	4.24	4.29	3.1	4.0	510	490
P_2	3.58	3.57	5.1	6.2	780	780
S_2	3.57	3.57	4.4	5.9	730	720
Cl_2	3.76	3.74	2.5	3.6	560	570

More to read

- Self-interaction correction
- The exchange-correlation-energy functional via the exchange-correlation hole
- The exchange-correlation-energy functional via wave-vector analysis



MOLECULAR PHYSICS, 2017
VOL. 115, NO. 19, 2315–2372
https://doi.org/10.1080/00268976.2017.1333644

Taylor & Francis
Taylor & Francis Group

TOPICAL REVIEW

OPEN ACCESS

Check for updates

Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals

Narbe Mardirossian[a] and Martin Head-Gordon[a,b]

[a]Kenneth S. Pitzer Center for Theoretical Chemistry, Department of Chemistry, University of California, Berkeley, CA, USA; [b]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Generalized gradient approximation (GGA)

$$E_x^{\mathrm{GGA}}[\rho] = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} \int d\mathbf{r}\, \rho^{4/3} F(s)$$

$$s = \frac{|\nabla\rho(r)|}{(2k_F\rho)}$$

$$k_F = (3\pi^2\rho)^{1/3}$$

$$F(s) = (1 + 1.296s^2 + 14s^4 + 0.2s^6)^{1/15}$$

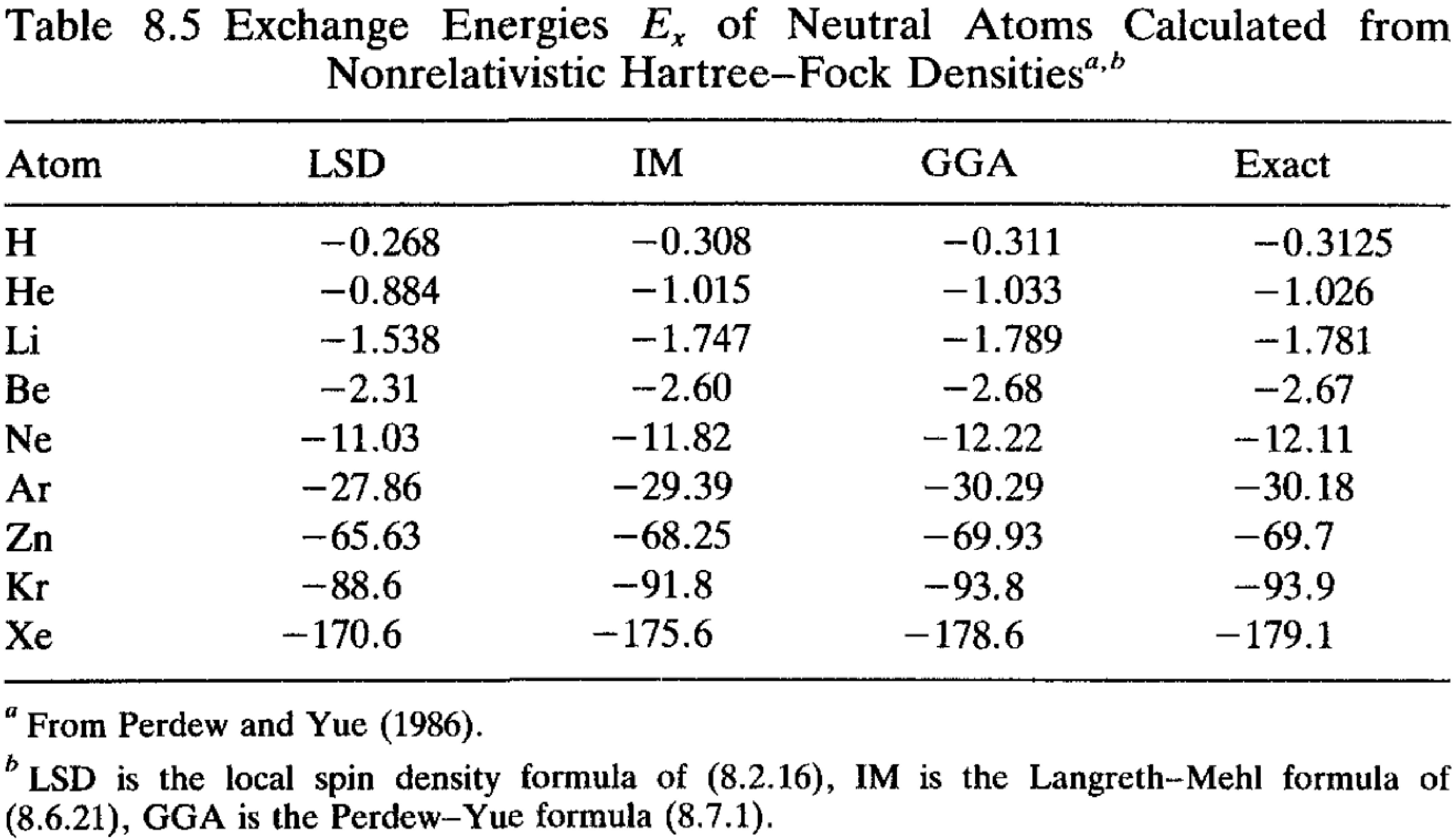


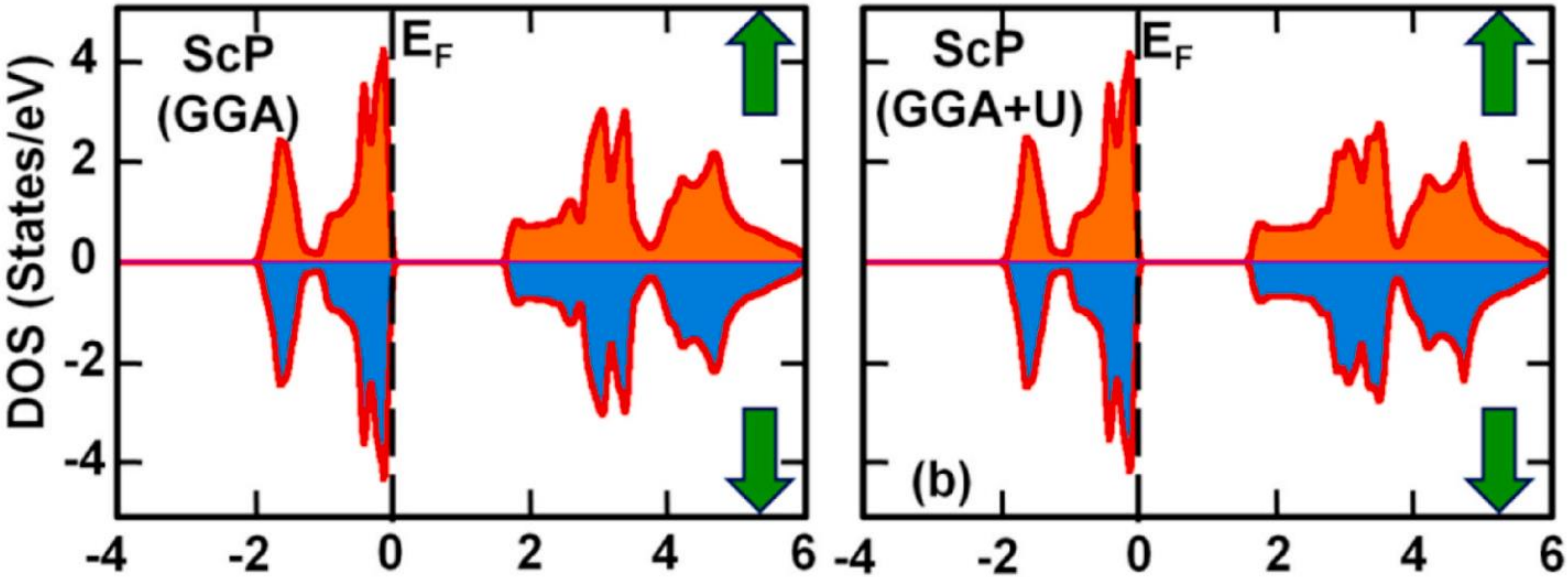
Table 8.5 Exchange Energies E_x of Neutral Atoms Calculated from Nonrelativistic Hartree–Fock Densities[a,b]

Atom	LSD	IM	GGA	Exact
H	−0.268	−0.308	−0.311	−0.3125
He	−0.884	−1.015	−1.033	−1.026
Li	−1.538	−1.747	−1.789	−1.781
Be	−2.31	−2.60	−2.68	−2.67
Ne	−11.03	−11.82	−12.22	−12.11
Ar	−27.86	−29.39	−30.29	−30.18
Zn	−65.63	−68.25	−69.93	−69.7
Kr	−88.6	−91.8	−93.8	−93.9
Xe	−170.6	−175.6	−178.6	−179.1

[a] From Perdew and Yue (1986).

[b] LSD is the local spin density formula of (8.2.16), IM is the Langreth–Mehl formula of (8.6.21), GGA is the Perdew–Yue formula (8.7.1).

I.U.N. Lone et al., Vacuum 191 (2021) 110328



A. Anjami et al.: Results Phys. 7 (2017) 3522–3529