Erratum to: Density Functional Theory

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The original version of this book was inadvertently published with errors. Those errors have been corrected as follows:

Chapter 5: Virial Theorems

Page 221

Equation (5.18) was revised. The quantities involved satisfy an inequality, rather than an equality.
The derivation of Eq. (5.18) was erroneously based on the implicit assumption that the total energy obtained from the scaled full wavefunction $|\Psi_{0,\lambda}\rangle$, Eq. (5.2), is identical with

$$E[n_\lambda] \;=\; T_\mathrm{s}[n_\lambda] + E_\mathrm{ext}[n_\lambda] + E_\mathrm{H}[n_\lambda] + E_\mathrm{xc}[n_\lambda]$$

not only for $\lambda = 1$, but also for $\lambda \neq 1$. The correct relation between these two energies [293] follows from the fact that the unscaled ground state $|\Psi_0\rangle = |\Psi_{0,\lambda=1}\rangle$ minimizes the expectation value $\langle\Psi|\hat{T} + \hat{W}|\Psi\rangle$, if $|\Psi\rangle$ is restricted to that part of the Hilbert space which gives the correct ground state density,

$$E_0 \;=\; \min_n \left\{ \min_{|\Psi\rangle\to n} \langle\Psi|\hat{T} + \hat{W}|\Psi\rangle + \int d^3r\, n(\boldsymbol{r})\, v_\mathrm{ext}(\boldsymbol{r}) \right\} .$$

As a consequence, the scaled state $|\Psi_{0,\lambda}\rangle$ minimizes $\langle\Psi_\lambda|\hat{T} + \lambda\hat{W}|\Psi_\lambda\rangle$. In fact, the scaling behavior of the expection values involved, Eqs. (5.7) and (5.13), directly leads to the relation

$$\langle\Psi_\lambda|\hat{T} + \lambda\hat{W}|\Psi_\lambda\rangle \;=\; \lambda^2\langle\Psi|\hat{T} + \hat{W}|\Psi\rangle .$$

The updated online versions of these chapters can be found at
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However, restricting $|\Psi\rangle$ on the right-hand side of this equation to give the correct ground state density automatically implies that the density is restricted to n_λ on the left-hand side (by construction of $|\Psi_\lambda\rangle$). Therefore $|\Psi_{0,\lambda}\rangle$ minimizes the expectation value on left-hand side [293], instead of minimizing $\langle\Psi|\hat{T}+\hat{W}|\Psi\rangle$. This result can then be combined with the Levy-Lieb constrained search definition of the density functional $F_{\rm LL}[n]$, Eq. (2.59). Since $F_{\rm LL}[n]$ minimizes the expectation value $\langle\Psi|\hat{T}+\hat{W}|\Psi\rangle$ for given constraint $|\Psi\rangle \to n$, one finds [293]

$$F_{\rm LL}[n_\lambda] \;\leq\; \langle\Psi_{0,\lambda}|\hat{T}+\hat{W}|\Psi_{0,\lambda}\rangle\,.$$

Decomposing $F_{\rm LL}$ as

$$F_{\rm LL}[n_\lambda] \;=\; T_{\rm s,LL}[n_\lambda]+E_{\rm H}[n_\lambda]+E_{\rm xc,LL}[n_\lambda]\,,$$

finally allows to establish an inequality for the correlation functional $E_{\rm xc,LL}[n]$ under scaling [293],

$$E_{\rm c,LL}[n_\lambda] \;\leq\; \lambda^2\left[\langle\Psi_0|\hat{T}|\Psi_0\rangle - T_{\rm s,LL}[n]\right]+\lambda\left[\langle\Psi_0|\hat{W}|\Psi_0\rangle - E_{\rm H}[n]-E_{\rm x,LL}[n]\right], \tag{5.18}$$

which has to replace the old Eq. (5.18). Note that this inequality is strict for $\lambda \neq 1$, while an identity is obtained for $\lambda = 1$. We thank Mel Levy for making us aware of this mistake.

Equation (5.18) was used to derive relation (5.35). However, Eq. (5.35) can also be established by combination of Eqs. (5.23) and (5.34), which are both independent of (5.18). Therefore Eq. (5.35) remains valid.

Page 224

The order of the equations (5.33), (5.34) and (5.35) was changed and all three equations were renumbered. The updated order is shown below.

Equation (5.33) (former 5.34):

$$\left.\frac{d}{d\lambda}E[n_\lambda]\right|_{\lambda=1} = 0\,,$$

Equation (5.34) (former 5.35):

$$\begin{aligned} 0 = {} & 2T_{\rm s}[n]+E_{\rm H}[n]+E_{\rm x}[n]-\int d^3r\, n(\boldsymbol{r})\,\boldsymbol{r}\cdot\boldsymbol{\nabla}v_{\rm c}(\boldsymbol{r}) \\ & +\langle\Psi_0|\hat{V}_{\rm ext}|\Psi_0\rangle+\sum_\alpha \boldsymbol{R}_\alpha\cdot\frac{\partial}{\partial\boldsymbol{R}_\alpha}\langle\Psi_0|\hat{V}_{\rm ext}|\Psi_0\rangle\Big|_{\rm expl.}\,, \end{aligned}$$

Equation (5.35) (former 5.33):

$$E_{\rm c}[n] = -\int d^3r\, n(\boldsymbol{r})\,\boldsymbol{r}\cdot\boldsymbol{\nabla}v_{\rm c}(\boldsymbol{r}) - T + T_{\rm s}[n]\,.$$

Chapter 8: Relativistic Density Functional Theory

Page 374

Equation (8.111) was revised: Since in the *no-pair* RDFT formalism we have chosen to subtract the rest mass from the energy, the occupation function has to be adjusted accordingly.

$$\Theta_k = \begin{cases} 0 \text{ for } \varepsilon_k \leq -2mc^2 \\ 1 \text{ for } -2mc^2 < \varepsilon_k \leq \varepsilon_\mathrm{F} \\ 0 \text{ for } \varepsilon_\mathrm{F} < \varepsilon_k \end{cases} .$$

Page 396

Table 8.6 was revised. The data for Au have been corrected and the updated version is shown below.

Atom	XRR	Nonrel. spin
Cr	1045942.2	1045942.0
Fe	1267116.4	1267116.2
Eu	10814457.4	10814456.1
W	16101781.8	16101781.8
Au	18966363.2	18966363.2
U	27925395.7	27925395.6
Am	30335910.7	30335910.3