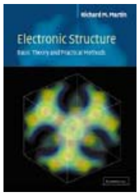

# **Electronic Structure: Basic Theory and Practical Methods,**

Richard M. Martin, Cambridge University Press, 2004.

## Errata

(May, 2005 -- only important errata listed – not minor typos)

xxi Notation: $u_{\alpha\beta}$ denotes a strain tensor (not a stress tensor)
2: line 6 – 1991 should be 1911
64: Eq. (3.48) – The large square brackets should be omitted.
70: Eq. (3.64) – indices *n* and *i* should be replaced by *m* as shown in the equation at the right:

$$\sum_{j=0}^{m} \langle \psi^{(j)} | \psi^{(m-j)} \rangle = 0, \; m \neq 0. \quad (3.64)$$

70: line after (3.64) should read:
where we have collected all terms of order $\lambda^m$ and then set $\lambda$=1.
72: Exercise 3.19 is incorrect as stated. The second sentence should read:
Show that such an empty orbital does not experience a self contribution to the exchange energy, whereas for a filled state there is an attractive self term in the exchange.
75: Caption of Fig. 2 – 60º should be replaced by 90º in two places.
83: Eq. (4.14) – for fcc, $\mathbf{b_3}$ should be (-1,1,1).
84: Eqs. (4.16) and (4.17) contain spurious "|;". These should be omitted.
97: Exercise 4.3 – "60 degrees" should be replaced by "90 degrees".
117: Exercise 5.14 – The hint should be replaced by:
(Hint: Assume the change in the density due to the impurity is $\delta$n(r) = exp(-$k_{TF}$ r)/r , and determine the decay constant $k_{TF}$ from the TF equations expanded to linear order in $\delta$n(r).)
127: Eqs. (6.20) - (6.22) – corrections as shown to the right:

$$\Omega[\hat{\rho}] = \mathrm{Tr}\hat{\rho}\left[(\hat{H} - \mu\hat{N}) + \frac{1}{\beta}\ln\hat{\rho}\right], \quad (6.20)$$

$$\Omega = \Omega[\hat{\rho}_0] = -\frac{1}{\beta}\ln \mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}, \quad (6.21)$$

$$\hat{\rho}_0 = \frac{\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}}. \quad (6.22)$$

137: Eq. (7.3) – the last term should be integrated over all space.
157: line before (8.11) – $n^{-1/3}$ should be $n^{1/3}$
189: Eq. (10.10) – in the last term $r^2$ should be $r^{-2}$
201: line above Eq. (10.40) – $\psi^2$ should be $\psi^1$
252: line 2 – Mathieu (instead of Matthew)
252: line 4 – Exercise 12.4 (instead of 12.7).
261: bottom – [567] (instead of [560])
287: Eqs. (14.15) and (14.16) – The x and y components should be interchanged to agree with the cell oriented as in Fig. 4.5 and 14.9a.
Two lines below (14.16) – the K point should be ($k_x$ = (2/3)(2 $\pi$/a), $k_y$ = 0).
296: Exercise 14.19 – The K point should be ($k_x$ = (2/3)(2 $\pi$ /a), $k_y$ = 0).
472: last sentence of section 23.7 – The reference should be to Haynes and Payne [859] see errata for the references.
479-80: Eqs. (B.4) and (B.5) should be omitted; they repeat (B.2) and (B.3) and contain small errors.
In Eq. (B.6) the letters "m" and "M" are spurious and should be omitted. In the first line of (B.6) n($r_s$) should be ln($r_s$) in both places. Note that only selected forms for the unpolarized case are given; complete expressions can be found in [224,368,413].
503: Eq. (F.7) – Replace by $\gamma_E$ = - $\alpha$ $(Ze)^2/(2R)$, where 2R = d, the nearest neighbor distance for ionic crystals (top line of Tab. F.1), and R = $R_{WS}$, the Wigner Seitz radius for elemental crystals (bottom line of Tab. F.1).
504: Replace the lines after Eq. (F.9) by:
which is very close to the Madelung energies for the close-packed metal in Tab. F.1.
575: The speed of light in atomic units is 137.036,000 (instead of 137,036,000 )

**References:** [859] P. D. Haynes and M. C. Payne, "Localised spherical-wave basis set for O(N) total-energy pseudopotential calculations", Comput. Phys. Commun. 102, pages 17-27 (1997).

**Back Cover: last sentence -** Recently he has been associate editor for condensed matter theory for the Reviews of Modern Physics condensed matter theory. (Peter Littlewood is now associate editor for condensed matter theory.)