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## Errata and Comments

***"Finite Element and Boundary Element Applications to Quantum Mechanics"***

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Some of the following comments are obvious, but I have listed all the comments, corrections, typos, errata that I have identified so far. I would be most grateful to the readers if they email me any comments, corrections or typos that are not listed below.– LRR

**Ch. 1:**

p14: Equation above (1.23) should read:

$$\delta A[q] = A[q+\delta q] - A[q] = \int dt' \frac{\delta L[q]}{\delta q(t')} \delta q(t').$$

**Ch. 2:**

p34: Just below Eq. (2.9), replace $\xi_\ell$ by $\xi_\ell^{(i_{el})}$.

p41: replace *n* by "*iel*" in Eqs (2.22) and (2.23). A simpler way to make the correction is to include a sentence above Eq.(2.22) stating, "In the following equations we replace *iel* by *n* for convenience of notation.

p47: In Equation (2.36) the right side should be $\left(\frac{m\omega}{\pi\hbar}\right)^{(1/4)} e^{-(m\omega x^2/2\hbar)}$.

p48: In Eq. (2.44) the functional is

$$J[\chi_{2s},\alpha] = -\frac{e^2}{a_0}\left[\frac{3\alpha-7\alpha^2}{6} + \frac{(\alpha^2/2)}{(\alpha^2-\alpha+1)}\right].$$

p49: Eq. (2.45) should read

$$\chi(\mathbf{r}) = \varphi(\mathbf{r}) - \sum_{i=1}^{n-1} \psi_i(\mathbf{r}) \int d^3r' \psi_i^*(\mathbf{r}')\varphi(\mathbf{r}')$$

**Ch.3:**

p78: In Eq. (3.28) a sum over *i* is understood. This is the usual Einstein convention of repeated indices having an implicit sum over them.

p79: Fourth line below Table 3.1: The sentence should read, "…eigenvalues obtained to five significant figures is 39."

**Ch. 5:**

p110: Equation (5.2), the left side does not need a subscript (I). It should read:

$V(x) = \ldots.$

Correspondingly, on p115, in the second line below the header for subsection 5.4.1 we need only *V*, and not $V_I$. Again in line 14 on p117, we need only *V* and not $V_I$.

p112: Equation (5.10), the second equation requires a factor $1/c^2$ on the right side so that we may use $m_e c^2 = 0.511 \times 10^6$ eV in the denominator and $\hbar c = 1.9732 \times 10^{-5}$ eVcm.

p112: Above Eq.(5.11), insert: “It is understood that in the following that we are using a dimensionless variable *x* and the *tilde* on *x* will be dropped.”

p116: Line 7 from the bottom: It might be clearer if we multiply by $\Phi_\beta$ rather than $\Phi_\alpha$ and go through the arguments in the following. Clearly, the sum over α in Eq. (5.24) is just a summation over a running index.

p117: On the last line, in the equation (no number) the left side should have $M_{\beta\alpha}$ .

p121: In Figure 5.2: the subscripts used in the right side of the displayed equation, for the quantity Q are interchanged: the column vector should have the entries: $\{A, -Q_{21}A, -Q_{31}A, -Q_{41}A, -Q_{51}A, 0\}$.

p127: Equation (5.37) should read:

$$V_a(x) = \begin{cases} V_1, & \text{for} \quad x < -d/2, \\ 0, & \text{for} \quad -d/2 < x < d/2, \\ V_3, & \text{for} \quad x > d/2 \end{cases}$$

and, correspondingly, Fig. 5.7 should have the coordinate labels (-d/2) and (+d/2) at the two sides of the quantum well.
Again, in Eq. (5.38) the last entry should be (+d/2).

p127: Figure 5.7 should have +d/2, *in the figure*, for the right boundary of the quantum well.

p127: Eq. (5.38) should have, for $x \le -d/2$ , the exponential to be $+\kappa_1 (x + d/2)$

p128: Insert after Eq. (5.41): “The wavefunction appearing in Eq. (5.41) is normalized over the entire physical structure.”

p129: Eq. (5.43) should have “$c_1$” replaced by “$c_3$”. In addition, on line 8 from the top, replace $c_1$ by $c_3$.

**Ch. 6:**

p149: Equation (6.1) should have $m^*_i$ being dependent on *z* and the order of the derivatives should be such that $1/m^*_i(z)$ occurs between the two derivatives *d/dz* acting on the wavefunction in the kinetic energy term.

Also, after Eq. (6.1), insert:
“The inplane dispersion is modified even in the one-band parabolic model in the layered heterostructures. So the inplane masses are complicated by this effect. Here we are simplifying the situation by assuming that the effective masses in the inplane direction are constant, and that their values in each layer correspond to the bulk values in the layers.”

p149: Equation (6.2) should have “f(z)”, with no tilde on z.

p150: Equation (6.3) should have the reduced energy ε to correspond to the energy ε(*z*) associated with the motion in the direct perpendicular to the planes.

p152: Equation (6.13) should have $m^*_i$ instead of just $m^*$ on the right side.

p152: Equation(6.13) and the equation above it should have n(z) on the left side, rather than a z with a tilde on top of it.

p154: Eq.(6.20), for T > 0K in the second line of the equation, should have no \ell_0 or m_0 in the denominator.

p157: Equation (6.26) should have a tilde on top of each occurrence of *d* on both sides of the equation. The same change is needed in line 6 below Eq.(6.26) and the following sentence.

p157: Equation (6.27) should have a negative (-) sign on the left side in order to be consistent with Eq.(6.28) on the next page.

p158: The occurrences of *d* in the text in the second paragraph require a tilde on top of *d.*

p159: Again in Equation (6.29) and below it, we need a *tilde* on top of *d.*

p160: Again in Equation (6.30) and below it, we need a *tilde* on top of *d.*

p164-165: In Sec. 6.5.4, we need a *tilde* on top of *d* for each occurrence of *d.*

p164: Equation (6.33) should read:

$$\delta A[V] = 0 = \int_{\tilde{d}_l}^{\tilde{d}_r} d\tilde{z} \left[ \frac{d}{d\tilde{z}} \left( \varepsilon(\tilde{z}) \frac{dV_{ch}(\tilde{z})}{d\tilde{z}} \right) - \left( S_D + S_e \right) \right] \delta V_{ch}(\tilde{z})$$
$$- \left[ \delta V_{ch}(\tilde{z}) \varepsilon(\tilde{z}) \frac{dV_{ch}(\tilde{z})}{d\tilde{z}} \right]_{\tilde{z}=\tilde{d}_r} + \left[ \delta V_{ch}(\tilde{z}) \varepsilon(\tilde{z}) \frac{dV_{ch}(\tilde{z})}{d\tilde{z}} \right]_{\tilde{z}=\tilde{d}_l} .$$

**Ch. 7:**

p174: The first factor of 2 on the right side in Eqs. (7.12)-(7.15) should be replaced by a sum over the spin $\sigma = \pm 1$. This is to allow for spin splitting in the magnetic field. Correspondingly the energies $E$, $E_n$ take on a spin index and should be $E_{n,\sigma}$.

p176: Sixth line from bottom of page: $R_0$ should have $B_0^{-1/2}$ to read:

"This leads to $R_0 = 256.56 A / [B_0]^{1/2}$ with $B_0$ in Tesla."

P187: In Eq. (7.27) the factor of $(1/2\pi^3)$ should be replaced by $1/(2\pi)^3$.

p189: The right side of Equation (7.32) has an exponent of (-2) on the quantity in the large parentheses.

p191: Remove the factor of $\hbar$ in the equation below (7.38), in Eq. (7.39), and in the equation in the line below it.

p192: Insert $\eta(\tilde{q}_x)$ just before the equality sign in Eq. (7.41).

**Ch. 9:**

p218: Equation (9.5): $N_3$ and $N_4$ are interchanged and need to be switched.

p 237: Equation (9.45) should have a factor ½ on the right side.
(Note that for $f(\xi,\eta) = 1$, we expect the sum over *w_i* to equal ½ for the area of a standard unit triangle.)

**Ch. 11:**

The energies in the Tables 11.2-11.5 are given in atomic units (Hartree) where 0.5 Hartree = 1 Rydberg. But the text says they are in Rydbergs instead of in Hartree units. For example, the field-free ground state has a binding energy 0.5 Hartree = 1.0 Rydberg.

The figure captions in Figs. 11.2 and 11.3 refer to B_0=2.35 $\times 10^9$G, This should be 4.70 x10^9G in the figures.

Note that the text and tables use $\gamma$. (Our PRA 40, 4777 (1989) paper used atomic units and $B_0$=2.35 $\times 10^9$G. In our Computers in Physics paper B was in units of 4.70$\times 10^9$G. )
Eq. (11.3) should have ....$\gamma\, m - \gamma$ +.., and not the plus sign it has.

**Ch. 13:**

P308: The last three equations, appearing in Equation (13.18), should have $y_1$ instead of $y_i$ on the right side (This should be as in the first equation.)

**Ch. 14:**

p349: Equation (14.64) has to be realigned.

**Ch. 15:**

p364: Figure 15.1: replace *9* by *11* in the figure caption.
p364: replace *9* by *11* on the last line in the page.

**Appendices:**

P515: In line 4, replace (A.18) by (A.19).
p519: The integral expression for Gauss-Chebychev formula should have the factor in the argument to be $\frac{1}{\sqrt{1-z^2}}$ , with $z$ replacing $x$.
p524: At the end of Problem 3: remove "Also, compare adaptive Gauss--Legendre quadrature with a straight application of Gauss-Hermite quadrature."
Here Gauss Hermite is not applicable since the range of the integration is not from -∞ to +∞.

p532: Just above Sec. B3: Insert:

Thus the integral representation of δ(x) is $\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\xi\, e^{i\xi x}$.

p534: The restriction below (B.23) is not needed since:

$$\int \theta'(x)\, f(x)\, dx = -\int \theta(x)\, f'(x)\, dx + (\theta(x) f(x))\,\Big|_{-\infty}^{\infty}$$

$$= f(\infty) - \int \theta(x)\, f'(x)\, dx = f(\infty) - \int_0^{\infty} f'(x)\, dx$$

$$= f(\infty) - f(\infty) + f(0) = f(0).$$

P537: In Problem B.2 the potential function should not have a delta-function. The presence of the delta-function changes the units since the function has units of inverse length.

p542: In Eq. (C.6), the integral should have *dx'*.

p547: 5th line from the bottom, replace *L* by *H.*

p550: Two lines above Eq. (C.32), the eigenvalues should read

$$-\lambda_n = k_n{}^2 = (n\pi / L)^2;\; n = 1,2,3,....$$

p582: Table D2: The value of the Bohr magneton should be 5.788..× $10^{-5}$ eV/T.