Errata (first printing) – Version 2: 10 August 2018

p. 2 — Sixth line of text, typo, should read “Friedrich” [Thanks Y. Yang]

p. 10. — Bottom of p.10 (second equation), \( \psi \) on LHS should have subscript “\( _n \)” [Thanks R. DiStasio]

p. 11 — In top equation of Eqn 1.6, \( \psi \) on LHS should have subscript “\( _n \)” [Thanks R. DiStasio]

p. 22 — (Newer versions of Mathematica enforce an ordering on integration and plotting operations that breaks this code.) In last code block, change “x” to “xx”. That is, code should read:

```mathematica
Plot[
    NIntegrate[Conjugate[equalSuperposition[xx, L, t]]*
        equalSuperposition[xx, L, t], {xx, 0, L}]
    ... etc.
```

Alternatively, one can circumvent this problem by defining the integral as a separate function, \( \text{intX[]} \), and then calling it as shown below:

```mathematica
hbar=1; m=1; L=5; (*define mass and length in atomic units*)

(*define the integral to plot*)
intX[L_, t_] := NIntegrate[Conjugate[equalSuperposition[x, L, t]]*
    equalSuperposition[x, L, t], {x, 0, L}] (*function performs integration*)

Plot[
    intX[L, t], {t, 0, 100},
    AxesLabel -> ... etc.
```

p. 38 -- first line of code. Missing "{" and "}" around first two arguments in Table[] function. Should read:

```mathematica
estate2withcoords = Table[{N[a*j], estate2[[j]]}, {j, 1, nPoints}];
```

p. 39 — To be completely analogous to the earlier code entry, the
second code entry should include the complex conjugation function, as shown:

Timing[ Conjugate[estate2].(xcoords*estate2)*a ]

(Note that this has no effect on the calculation because all the entries in the eigenvector are real.) [Thanks R. Macrae]

p. 52 — In Eq. 3.6, the term [E- V_j] should be [V_j - E]. [Thanks R. Macrae]

p. 64 — Problem 3-7, units in grid specification are incorrectly specified in terms of the realspace grid spacing, when what is intended is the sampling of kinetic energy points. Should read: “sample the transmission as a function of kinetic energy at intervals $\Delta E = 0.001$, $E_{h}$… sample at intervals $\Delta E = 0.1$, $E_{h}$”

p. 70 — Above last section of code. There are in fact “six parameters”, and not “five parameter” as stated in the text. [Thanks R. Macrae]

p. 72-73 — The default NMinimize[] settings in Mathematica 11.1.1.0 find a slightly lower minimum. The outputs for the remainder of this subsection read, in order:

{0.197401, {a -> -0.0000120652, b -> 22.719, c -> 0.908926, d -> -2.2186, e -> 0.238221, f -> -0.00252193}}

0.00469079

{0.197401, {a -> -0.0000120652, b -> 22.719, c -> 0.908926, d -> -2.2186, e -> 0.238221, f -> -0.00252193}}

{a -> -0.0000120652, b -> 22.719, c -> 0.908926, d -> -2.2186, e -> 0.238221, f -> -0.00252193}

a -> -0.0000120652

-0.0000120652

p. 80 — The fifth term in the output for increasingBasis should read “0.433845” [Thanks R. Macrae]

p. 85 — The terms on the right hand side of Eq. (4.25) should all have the numerator $L^{(1 + 2i + 2j)}$. Alternatively, the right hand
side of this equation can be written more compactly as:
\[
\frac{(3 i+3 j+2) \ L^2 \ (i+j+1) \ (i+2 \ j+1) \ \ (2 i+2 \ j+1)}{(i+j+1) \ (2 i+j+1) \ \ (i+2 \ j+1) \ (2 i+2 \ j+1)}
\]
[Thanks R. Macrae]

p. 95 — In Problem 4-9 (d), exact value is “−2.903724375”.

p. 110 -- The second term in the output of evals, is incorrect. The first output on this page should read:

\{-0.917935, \ 2.05685\}

p. 119 — In definition of twoElecInt[], the first propK[] function is missing the closing “}”. The function should read:

twoElecInt[alpha_,rA_,beta_,rB_,gamma_,rC_,delta_,rD_] :=
propK[alpha,rA,beta,rB]*propK[gamma,rC,delta,rD]*
... etc.

p.178 — expand name (better Chinese orthography), to: “postdoctoral fellow Lu Jeu Sham” [Thanks Y. Yang]

p. 181 — In last line of code on this page, the argument should be 100, not 10. This last line should read:

ringLineComparison[100]} ]

p. 189 — Code input at bottom of page is unnecessarily printed twice.

p. 190 — In first line of code output on page should read: \{-3, \ 3\}

p. 202— Fact check correction: “the first Nobel Prize awarded to a Japanese chemist” [Thanks Y. Yang]

p. 367 — The data supplied in the first line of code displays the L=11 case, but should display the L=9 case. This first line should read:

ListPlot[calcGr[coordList9, 9.], 0.01], ... etc.

p. 375 — Missing "{" in last argument of NDSolve[], second line of code on this page. Line should read:

soln1 = NDSolve[ {a'[t] == -k1*a[t], a[0] == 1}, a, \{t, 0, 10\}][[1]]

p. 409 — Code output lines after the inputs ?x and ?z should read:
Global \( x \) and Global \( z \), respectively.

p. 426 — In problem A-2, second line delete “2” superscript. Should read, “and principal quantum number \( n \). (Recall: …”

p. 428 — In the first sentence of problem A-15, only one \( f(x) \) should be present in the integrand. [Thanks R. Macrae]

p. 440 — In data table for Problem B-1, the value of the molar heat capacity at \( T = 1000K \) should read \( 45.98 \)

p. 443 — In Problem B-8, part (b), modify inline equation to read \( PM/(\rho RT)-1 \)

p. 447 — Output towards bottom of page should be changed from “01.” to “0.1”