Solutions practice test

The problem:

You are given a particle in a finite square well (shown below) with width of 10 length units, i.e. \( a = 10 \). This problem is different than the particle in a box we have studied, in that the potential outside the box is finite, in this case, 2 Rydbergs (Ry). I have chosen to work in units of Ry for in these units \( \hbar = 1 \) and an electron has mass \( = 1 \).

Now suppose there is an electron in this box and you want to find something out about the energy, momentum, or position of this electron when it is in one of its first three quantum states. Well, you could solve the Schrödinger equation. Or you could take the easier way and go to Quantum Depot where they will sell you the first three wave functions to this problem.

You get access to these wavefunctions by initializing the cell below. Though the cell looks really complicated, you don't care as the first three wave functions for an electron in the above potential will be at you disposal through the functions \( \text{wf}[1] \), \( \text{wf}[2] \), and \( \text{wf}[3] \). Note you did not pay enough to get higher wavefunctions i.e. \( \text{wf}[4] \) etc. So don't go looking for them. It will just frustrate you.

Also as an added bonus you get the potential function for free. It is called \( \text{vfsw} \) (potential finite square well).
Warm up (Note these problems refer to our regular particle in a box problem--a particle in an infinite square well)

1. Write down the Hamiltonian for a free particle of mass m constrained to lie along the x-axis between x=0 and x=a.

\[ -\frac{(\hbar)^2}{2m} \frac{d^2}{dx^2} \]

2. Write down \( \psi_1 \) for the particle in a box.

\[ \sqrt{\frac{2}{a}} \sin(\pi /a) \]

3. Plot \( \psi_1 \) for the particle in a box. Use a=10. Plot the probability density of \( \psi_1 \).

4. arb is made from a linear combination of the first three particle in a box wavefunctions. Find the three coefficients.

\( \left\{ \frac{1}{\sqrt{5}}, \frac{\sqrt{5}}{6}, \frac{\sqrt{5}}{8} \right\} \)

Now for the harder questions: The Particle in a Finite Square Well

5. Plot the potential (vfsw) for x between -4 and 14.
6. Plot the \( \psi[1] \) and the probability density of \( \psi[1] \) between -4 and 14 on the same plot. Is there a probability of finding a particle in this state outside the box?

7. Show that \( \psi[1] \), \( \psi[2] \), and \( \psi[3] \) are orthogonal. (Think, given what you learned from the above exercises, what will be the limits on your overlap integral? And note, they gave you numerical solutions at Quantum Depot, so you might expect some roundoff error.)

They are orthogonal—see below


Yes

10. Calculate the probability that a particle in each state—\( \psi[1] \), \( \psi[2] \), or \( \psi[3] \)—is outside the box.
Now for the harder questions:
The Particle in a Finite Square Well

5. Plot the potential \(v_{fsw}\) for \(x\) between -4 and 14.

<table>
<thead>
<tr>
<th>x</th>
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<tbody>
<tr>
<td>0</td>
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<td>9</td>
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<td>10</td>
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6. Plot the \(w_{f[1]}\) and the probability density of \(w_{f[1]}\) between -4 and 14 on the same plot. Is there a probability of finding a particle in this state outside the box?

5 10
0.5
1.0
1.5
2.0

7. Show that \(w_{f[1]}\), \(w_{f[2]}\), and \(w_{f[3]}\) are orthogonal.

\[ pib\psi[n_, a_] := \sqrt{\frac{2}{a}} \sin \left( \frac{n \pi x}{a} \right); \]
\[ s[f_, g_] := \int_{-a}^{a} f g \, dx; \]
\[ pibS[f_, g_, a_] := \int_{0}^{a} f g \, dx; \]

(* 3 and 3b *)
Plot[{pib\psi[1, 10], pib\psi[1, 10]^2}, {x, 0, 10}, PlotStyle -> Thick]

0.00212579, 0.0086633, 0.0203042 respectively

11. For a particle in the \(w_{f[2]}\) state, calculate its average kinetic energy. (Note: in the units you are using \(\frac{\hbar^2}{m} = 1\))

0.143159 Ry

12. For a particle in the \(w_{f[2]}\) state, calculate its average potential energy.

0.0173666 Ry

13. For a particle in the \(w_{f[2]}\) state, calculate its total energy.

0.160525 Ry

14. Are the results you found consistent with classical mechanics?

No! A particle with total energy = .16 Ry cannot move into a region where the energy barrier is 2 Ry
(* 4 *)

Table[pib[arb, pib[n, 10], 10], {n, 1, 3}]

\[\left\{\frac{1}{\sqrt{5}}, \frac{\sqrt{5}}{6}, \frac{\sqrt{5}}{8}\right\}\]

(* This is the right answer. Why are these coefficients different than those I used to define arb? *)

(* 5 *)

Plot[vfsw, {x, -4, 14}, PlotStyle -> {Thick, Red}]

(* 6 *)

Plot[{wf[1], wf[1]^2}, {x, -4, 14}, PlotStyle -> Thick]

(* Answers to 7 and 8 -- or you could do it by using the overlap integral nine times. Don't ask me what Chop does until you have checked out the Help menu *)

TableForm@Table[Chop[s[wf[n], wf[m]], 10^-5], {n, 1, 3}, {m, 1, 3}]
(* probability of being outside box *)

\[ \text{pob}[f_] := s[f, f] - \int_0^{10} f f dx \]

(* 10 *)
Table[pob[wf[n]], {n, 1, 3}]
{0.00212579, 0.0086833, 0.0203042}

(* 11 *)
\[ \text{avKe} = s[wf[2], \frac{-\partial_{x,z}wf[2]}{2}] \]
0.143159

(* 12 *)
\[ \text{avPe} = s[wf[2], v\text{fsw}wf[2]] \]
0.0173666

(* 13 *)
\[ \text{totalE} = s[wf[2], \frac{-\partial_{x,z}wf[2]}{2} + v\text{fsw}wf[2]] \]
0.160525

(* just to check *)
Chop[avKe + avPe - totalE]
0