A developmental research on introducing the quantum mechanics formalism at university level

Koopman, L.

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Chapter 9

Retention of Quantum Mechanical Concepts

This chapter describes the development of a test to 1) measure meaningfully learned basic quantum concepts and 2) measure the retention of these concepts. In education, a retention test aims at measuring to what extent learned content is retained in memory. Typically, a retention test is conducted twice, with a suitable amount of time between them. Comparing the test results of the two attempts enables to draw conclusions about what is retained in memory. The test was developed for the two courses that were followed in this research (QC and QP). Because the course content differed significantly, two separate tests were developed, one for each course. The QP retention test was conducted in 2006 and 2007, the QC retention test in 2007 and 2008.

There are two reasons to develop a retention test for this research. Observations in the Quantum Physics (QP) course gave the impression that much of the tutorial session work focused on performing calculations. The final exam reflects this. As a result students also seemed to focus on learning to perform the calculations. An important portion of the problems used in the tutorials were set up such that they might be made using “tricks”, or heuristic rules, rather than relying on understanding. In other words, students might be using rote learning techniques to perform the tasks given. In the Quantum Chemistry (QC) course students also appeared to rely on rote learning techniques, although with another reason. Students were found to experience great difficulties learning the material in a meaningful way. As a strategy to pass the final exam, some students seemed to fall back to learning it rotely. A retention test might reveal to what extent students in both courses learn the material meaningfully.

Another reason to develop a retention test is to compare interventions in successive years for both courses (see for instance [Kvam 2000]). Typically, in a null round, the retention rate is measured and compared to the retention rate the following year in which a set of interventions is implemented. Comparing
Chapter 9. Retention of Quantum Mechanical Concepts

the retention rate between the two years, might reveal whether there is a positive effect of the interventions on meaningful learning. Furthermore, the tests score can be compared to the exam score to reveal possible differences in what is tested.

9.1 Research questions

We pose the following three research questions:

1. What is the retention of quantum mechanics concepts based on the developed test?

2. Does the developed retention test measure meaningfully learned content?

3. How do the grades of the first attempt of the retention test compare to the grade of the course’s final exam?

From the theoretical background we will see that the first two questions are related. Regarding the third question: we would like to know how students perform on questions that test basic quantum concepts. We consider the concepts basic in the sense that they are the minimum we would like students to learn from the course.

9.2 Theoretical background

As explained in Chapter 3, Ausubelian learning theory distinguishes between two dimensions of learning: reception versus autonomous discovery learning and rote versus meaningful learning (Ausubel, Novak, & Hanesian, 1978). This latter dimension refers to the cognitive process that occurs within the learners mind. Meaningful learning is further explained by assimilation theory. In short meaningful learning requires new content to be connected in a meaningful way to existing cognitive structures. Contrary to this, rotely learned content exists relatively isolated in cognitive structure. This has an important effect on the retention of learned content.

Retention of rotely learned materials is influenced primarily by the interfering effects of similar rote materials learned immediately before or after the learning task. […] Retention of meaningful learned materials is influenced by properties of those relevant and cumulatively established ideational systems with which the learning task interacts and that determine its dissociability strength.

Ausubel et al. (1978, p. 144, paraphrased)

1 The concept dissociability strength refers to the process where a newly learned concept a is linked to an existing concept A, such that they become connected as A′a′, where the prime is to indicate that their meaning is changed as a result of their interaction. The dissociability strength now expresses how easily these two concepts can be recalled from memory as a′ and A′. As time passes, it will become less easy to recall a′, and what is left is the altered concept A′.
From the above we can conclude that meaningfully learned content is better retained than rote-ly learned content. As a corollary: the higher the retention rate the more meaningful the materials have been learned. Meaningful learning can be tested "by phrasing the test in a different language and presenting the test in a somewhat different context than the original learning material" Ausubel et al. (1978, p. 147, paraphrased). An alternative way to measure whether meaningful learning has taken place, proposed by Ausubel et al. (1978), is to present the learner with a follow-up learning task that can only be mastered if the previous learning task is genuinely understood.

It is to be expected that content learned more rote-ly is forgotten sooner than content learned more meaningfully. Ausubel et al. (1978) report on studies that found a time span of hours for nonsense syllables (Ebbinghaus, 1913) and days for poetry (Boreas, 1954). In a more recent literature review, Custers (2010) concludes that approximately two-third to three-fourth of knowledge will be retained after one year. This will drop to slightly below fifty percent in the next year.

Ausubel suggests that single facts are not recalled as well as abstract concepts that are strongly linked within cognitive structure. More recent research in memory and retention does not agree upon what is actually stored in memory: single facts, or abstract concepts. Bahrick (1984) claims that specific knowledge is stored and retrieved. Schema theory, on the other hand, claims that a general abstract schema is stored in memory, from which specific knowledge is reconstructed. From this theory it should follow that specific facts, and for instance names, are less well remembered than general facts and concepts. Neisser (1984) Cohen (1990) Conway, Cohen, & Stanhope (1991). Experimental results, however, do not consistently support this theory (Conway et al., 1991). Semb and Ellis (1994) provide a different perspective and emphasize that the degree of organization and integration of the content is important for recall. They hypothesize that a more integrated domain, with more connections or associations between items of knowledge, increases the probability that a given item will be remembered. This idea overlaps with what Ausubel claims. It remains unclear whether the abstractness of the knowledge is of influence on retention.

9.3 Methodology

9.3.1 Development of the test

One of the aims of the retention test was to measure understanding. To that end it consisted of two parts. The first part was made up of open ended questions in which students have to perform basic calculations and interpret their results. These questions were in part based on questions from the tutorial sessions and set up such that students did not have to rely on the memorization of rules, or formula’s (e.g. the Schrödinger equation). The second part of the test consists of six 3-tier, multiple choice questions adapted from the
Quantum Mechanics Visualization Instrument (QMVI, Cataloglu & Robinett, 2002). In these questions students have to interpret a graphical representation of the wave function, or the probability density. It has been found that multiple choice questions measure recall as well as recognition (Arzi, Ben-Zvi, & Ganiel, 1986). In essence our retention test should measure recall, not recognition. The multiple choice questions we used are suitable for this, because the options given are possible outcomes of a calculation, which cannot be recognized. There is only a possibility that students will revise their answer if for instance they see that the answer they would like to give is not one of the options.

The test was validated by asking feedback from the lecturers and a teacher of the problem solving sessions. Furthermore, some second-year students were asked if they thought the phrasing of the questions was clear. They also informally tried to make the test. Finally, structured interviews were held with three first-year students (one at a time). They were asked to make the test and think aloud. Based on these interviews we could determine whether the phrasing of the test questions was clear and whether students interpreted them as intended.

9.3.2 Sample selection and data collection

The retention test for QP was conducted in 2006 and 2007, for QC in 2007 and 2008. The first attempt was one month after the final exam, at a suitable moment during a practical (with permission of the responsible teacher). The second attempt was seven months after the final exam. For QC the second attempt was planned during a tutorial session of another course, for QP during the first tutorial session of the follow-up quantum physics course. For both attempts, students were not informed that there would be a test. Students were given enough time to finish the test (approximately 40 minutes). Between both attempts students have not received any formal instruction in quantum physics. Because we want to measure retention of concepts learned during either of the two courses (research question 2), we only include students in the analysis who have followed the course for the first time and have passed the final exam (grade 5.5 or higher).

To prevent a (literal) learning effect of the first attempt, two slightly different versions (A and B) of the test were used. These versions should be equally difficult such that their test scores can be compared. To determine whether both versions can be compared the students were divided into two groups. One group made version A of the test on the first attempt and version B on the second attempt. For the other group the order was reversed: first version B, then version A. This results in the scheme as shown in Table 9.1. In this Table A_{12} is for instance the average grade of group one on the second attempt, for version A of the test.

Following Ellermeijer (1987), a measure \( m \) is introduced to determine the extent to which the two versions of the test differed in difficulty. The measure
Table 9.1: The table shows which version of the test (A or B) was given to which group on the two attempts. A_{12}, for instance, is the average grade of group one on the second attempt, for version A of the test.

<table>
<thead>
<tr>
<th>group</th>
<th>attempt</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>11</td>
<td>12</td>
</tr>
<tr>
<td>2</td>
<td>B</td>
<td>21</td>
<td>22</td>
</tr>
</tbody>
</table>

\( m \) is defined as:

\[
m = \frac{(A_{11} + A_{22}) - (B_{21} + B_{12})}{2}.
\] (9.1)

A positive \( m \)-value indicates that version B is more difficult than version A. We have used \( m \) to correct for this difference in difficulty, by adding \( m \) to the test results for version B.\(^2\) In order to compare versions A and B of the test \( m \) should be small, typically within the standard deviation of the test results.

Furthermore, we do not want that the two groups, defined above, differ too much. To determine possible group differences a measure \( g \) is introduced, defined as:

\[
g = \frac{(B_{21} + A_{22}) - (A_{11} + B_{12})}{2}.
\] (9.2)

A positive \( g \)-value indicates that group 2 has better test results than group 1.\(^3\) Again, \( g \) should be small.

Table 9.2 shows the \( m \) and \( g \) values for both courses. We consider all these values small enough to enable comparison of versions A and B of the test for both groups. In the following the results are presented for the two groups combined, where we have corrected for a difference in test difficulty using the measure \( m \), as described above.

Because not all students have participated in both attempts of the test, we can define two samples. The retention sample consists of all students who have made both retention tests. The control sample consists of all students who have not made both retention tests (i.e. one, or none).\(^4\) We cannot control these samples completely, but we would like to know whether the retention sample is a representative draw from the total population.

Table 9.3 compares the final exam grades of both samples for both courses respectively. For the QC course the average exam scores in both 2007 and 2008

\(^2\)If we then recalculate \( m \) with the corrected test results, \( m \) will be zero.

\(^3\)The \( g \)-value is not altered when correcting for the difference in difficulty between test versions.

\(^4\)Thus, the total population of students that have passed the exam is the sum of both samples.
of both samples (retention and control) do not differ significantly \((p \gg 0.05,\) two-tailed t-test). This suggests that the retention sample is a representative draw from the student population. For the QP course the average exam scores in 2007 for both samples (retention and control) do not differ significantly \((p \gg 0.05,\) two-tailed t-test). Again, this suggests that the retention sample is a representative draw from the student population. However, in 2006 there is a small, but significant, difference \((p = 0.02,\) two-tailed t-test). The retention sample appears to be slightly better than the control sample.

Table 9.2: Comparison of versions and groups: \(m\) is a measure for the difference in difficulty, \(g\) is a measure for the difference between groups.

<table>
<thead>
<tr>
<th>Quantum Chemistry</th>
<th>2007 ((N_A = 3, N_B = 5))</th>
<th>2008 ((N_A = 2, N_B = 4))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m)</td>
<td>-0.10</td>
<td>-0.05</td>
</tr>
<tr>
<td>(g)</td>
<td>0.16</td>
<td>-0.70</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Quantum Physics</th>
<th>2006 ((N_A = 7, N_B = 9))</th>
<th>2007 ((N_A = 8, N_B = 9))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m)</td>
<td>0.22</td>
<td>0.23</td>
</tr>
<tr>
<td>(g)</td>
<td>0.36</td>
<td>-0.07</td>
</tr>
</tbody>
</table>

Table 9.3: Sample size and exam grade averages (SD) for the two years under consideration for both the retention and control sample. The mentioned p-values are for a two tailed t-test.

<table>
<thead>
<tr>
<th>Quantum Chemistry</th>
<th>2007</th>
<th>2008</th>
</tr>
</thead>
<tbody>
<tr>
<td>sample</td>
<td>grade N</td>
<td>grade N</td>
</tr>
<tr>
<td>retention</td>
<td>6.9 (0.7) 8</td>
<td>7.0 (1.2) 6</td>
</tr>
<tr>
<td>control</td>
<td>6.8 (0.9) 7</td>
<td>6.3 (0.5) 9</td>
</tr>
<tr>
<td>p-value</td>
<td>0.32</td>
<td>0.39</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Quantum Physics</th>
<th>2006</th>
<th>2007</th>
</tr>
</thead>
<tbody>
<tr>
<td>sample</td>
<td>grade N</td>
<td>grade N</td>
</tr>
<tr>
<td>retention</td>
<td>7.6 (0.9) 16</td>
<td>7.5 (1.0) 17</td>
</tr>
<tr>
<td>control</td>
<td>6.9 (0.9) 21</td>
<td>7.9 (1.3) 11</td>
</tr>
<tr>
<td>p-value</td>
<td>0.02</td>
<td>0.41</td>
</tr>
</tbody>
</table>
9.4 Results

In the next two sections we present the results of the retention test and compare the test results to the final exam grades. Because no significant intervention was planned for QP in 2007, the test cannot be used to measure an effect of such an intervention. After 2007 there was a new lecturer for QP and the research focused on QC from there on. The idea to do the same test for QC came after we had already implemented an important intervention in that course. Hence, a null measurement is missing. The retention test can thus not be used to compare the conventional course to an experimental course.

9.4.1 Quantum Chemistry

The results are represented graphically in Figure 9.1, which shows scatter plots comparing the first retention test attempt to the final exam (left scatter plot) as well as comparing both retention test attempts (right scatter plot) for both years under consideration.

Table 9.4 shows that in both years (2007 and 2008) the retention test score is significantly lower than the final exam grade ($p = 0.001$ resp. $p = 0.01$, two-tailed t-test). In 2007 there is non-significant, weak correlation between exam and retention test scores ($r = 0.59$, $p = 0.06$, one-tailed t-test). In 2008 the correlation is significant ($r = 0.81$, $p = 0.03$, one-tailed t-test). Although the 2007 correlation is weak, we conclude two things from these results. First, the retention test has similar discriminative power as the final exam: it distinguishes high achieving from low achieving students. Secondly, the test seems to test the same thing (i.e. “quantum mechanics”). As the retention test was designed to measure basic quantum concepts taught in the QC course, the low average test score is somewhat disappointing. It shows that students’ conceptual understanding of the course content is weak.

Table 9.5 compares the first and second attempt of the retention test. The test scores between the two attempts do not differ significantly. In other words: students’ performance does not improve nor decline between the two attempts. Based on the theoretical framework, we conclude that the test measures meaningfully learned content. Of course, the low $p$-value might also mean that we are unable to determine an existing difference due to the small $N$ in these samples.
Figure 9.1: QC retention 2007 (top, $N = 8$) and 2008 (bottom, $N = 6$) test results.
Table 9.4: Averages for the first attempt of the retention test and the final exam for the QC course. The p-values for the average grades are for a two tailed t-test. The p-values for the correlation coefficients are for a one tailed t-test.

<table>
<thead>
<tr>
<th></th>
<th>2007 (N = 8)</th>
<th>2008 (N = 6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>exam (SD)</td>
<td>6.9 (0.7)</td>
<td>7.0 (1.2)</td>
</tr>
<tr>
<td>attempt 1 (SD)</td>
<td>4.9 (1.2)</td>
<td>5.8 (1.1)</td>
</tr>
<tr>
<td>p-value</td>
<td>0.001</td>
<td>0.01</td>
</tr>
<tr>
<td>correlation</td>
<td>0.59</td>
<td>0.81</td>
</tr>
<tr>
<td>p-value</td>
<td>0.06</td>
<td>0.03</td>
</tr>
</tbody>
</table>

Table 9.5: Average values for the first and second attempt of the test (QC course). P-values for averages on a two tailed t-test, p-values for correlation on a one tailed t-test.

<table>
<thead>
<tr>
<th></th>
<th>2007 (N = 8)</th>
<th>2008 (N = 6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>attempt 1 (SD)</td>
<td>4.9 (1.2)</td>
<td>5.8 (1.1)</td>
</tr>
<tr>
<td>p-value</td>
<td>0.95</td>
<td>0.26</td>
</tr>
<tr>
<td>correlation</td>
<td>0.58</td>
<td>0.14</td>
</tr>
<tr>
<td>p-value</td>
<td>0.066</td>
<td>0.40</td>
</tr>
</tbody>
</table>
9.4.2 Quantum Physics

The results are represented graphically in Figure 9.2, which shows scatter plots comparing the first retention test attempt to the final exam (left scatter plot) as well as comparing both retention test attempts (right scatter plot) for both years under consideration.

Figure 9.2: QP retention 2006 (top, \( N = 16 \)) and 2007 (bottom, \( N = 17 \)) test results.

Table 9.6 shows that in both years (2006 and 2007) the retention test score is significantly lower than the final exam grade (\( p \ll 0.05 \), two-tailed t-test). In 2006 there is non-significant, weak correlation between exam and retention test scores (\( r = 0.40 \), \( p = 0.06 \), one-tailed t-test). In 2007 the correlation is significant (\( r = 0.72 \), \( p \ll 0.05 \), one-tailed t-test). As in the case of QC we conclude that 1) the retention test has the same discriminative power as the
final exam, and that 2) the retention test measures the same thing as the final exam. Again we see that the average retention test score is much lower than the average grade for the final exam. Thus, also for QP, students’ conceptual understanding of the course content is weak.

Table 9.7 compares the first and second attempt of the retention test. The test scores between the two attempts do not differ significantly ($p \ll 0.05$, two-tailed t-test). In this case the samples appear to be large enough. In other words: students’ performance does not improve nor declines between the two attempts. This result is consistent with the QC result. Thus, also the retention test for QC measures meaningfully learned content.

Table 9.6: Averages for the first attempt of the retention test and the final exam for the QP course. The p-values for the average grades are for a two tailed t-test. The p-values for the correlation coefficients are for a one tailed t-test.

<table>
<thead>
<tr>
<th></th>
<th>2006 (N = 16)</th>
<th>2007 (N = 17)</th>
</tr>
</thead>
<tbody>
<tr>
<td>exam (SD)</td>
<td>7.6 (0.9)</td>
<td>7.5 (1.0)</td>
</tr>
<tr>
<td>attempt 1 (SD)</td>
<td>5.7 (1.3)</td>
<td>5.8 (1.1)</td>
</tr>
<tr>
<td>p-value</td>
<td>$\ll 0.05$</td>
<td>$\ll 0.05$</td>
</tr>
<tr>
<td>correlation</td>
<td>0.40</td>
<td>0.72</td>
</tr>
<tr>
<td>p-value</td>
<td>0.06</td>
<td>$\ll 0.05$</td>
</tr>
</tbody>
</table>

Table 9.7: Average values for the first and second attempt of the test (QP course). P-values for averages on a two tailed t-test, p-values for correlation on a one tailed t-test.

<table>
<thead>
<tr>
<th></th>
<th>2006 (N = 16)</th>
<th>2007 (N = 17)</th>
</tr>
</thead>
<tbody>
<tr>
<td>attempt 1 (SD)</td>
<td>5.7 (1.3)</td>
<td>4.5 (1.7)</td>
</tr>
<tr>
<td>attempt 2 (SD)</td>
<td>5.5 (1.0)</td>
<td>4.8 (1.3)</td>
</tr>
<tr>
<td>p-value</td>
<td>0.46</td>
<td>0.23</td>
</tr>
<tr>
<td>correlation</td>
<td>0.44</td>
<td>0.85</td>
</tr>
<tr>
<td>p-value</td>
<td>0.04</td>
<td>$\ll 0.05$</td>
</tr>
</tbody>
</table>


9.5 Conclusion

Two retention tests were set up for two introductory courses on quantum mechanics to measure the retention of quantum concepts. The tests focus on conceptual understanding, rather than reproduction of procedures (e.g. solving the Schrödinger equation) and recall of learned facts (e.g. knowing the energy levels for atomic hydrogen). The QP retention test was conducted in 2006 and 2007, the QC retention test in 2007 and 2008. We answer the three research questions.

1. **What is the retention of quantum mechanics concepts based on the developed test?**
   For both courses, for all years there is no significant decline, nor improvement of test results within the chosen retention interval approximately six months.

2. **Does the developed retention test measure meaningfully learned content?**
   Literature on learning suggests that retention of concepts depends on the degree of connectedness of these concepts. For instance, roteley learned content will hardly be connected to what a subject already knows, while meaningfully learned content will be strongly connected to existing cognitive structures. As the retention is constant (research question 1), we conclude that the retention test (mainly) measures meaningfully learned content.

3. **How do the grades of the first attempt of the retention test compare to the grade of the course’s final exam?**
   For both courses, for all years, the average retention test score was significantly lower than the average exam score. Thus students performed less well on the content we tested. This difference can in part be explained by the fact that students were asked to make the test without notice during other curricular activities. However, our impression is that they took the test seriously. As the retention test was designed to measure meaningfully learned, core concepts taught during the courses, we conclude that students do not master these concepts at the level we would like. Furthermore, the final exams are unable to distinguish this lack of mastery.

9.6 Discussion

The main problem in conducting this test was the small number of participants, especially for the QC course ($\approx 7$). The maximum number of students will remain small, as there are approximately 30 first year students enrolled for QC and 60 for QP. Furthermore, we only want to include students that have passed for the final exam (typically $\approx 70\%$), resulting in even lower numbers. However, the response rate might be improved by using the final exam as a retention test. The final exam itself then is a null retention test. A second retention test can be made by repeating part of the final exam. Retention is then measured by comparing a selection of the exam items to the repeated test results. This second attempt should be incorporated in an activity that is obligatory for students.
9.A  Retention tests

The retention test for Quantum Chemistry is reproduced on pages 198–202. The retention test for Quantum Physics on pages 203–207. Both tests were translated from Dutch. The first question of each test is similar to the problems given during the tutorial sessions. Questions 2–7 are multiple choice questions adapted from the QMVI (Cataloglu 2002). Each of these questions ask the students to give a short motivation and indicate how certain they are of their answer (4-point Likert scale, ranging from −2 for very uncertain, to +2 for very certain). The students’ motivation and certainty were only used in the qualitative analysis of the test results.
Question 1: Bonding of H and F

In this problem we use the LCAO-MO approximation to study how the atoms H and F form the molecule HF.

a) In the scheme below, the lowest energy levels are given for H and F. The energy levels for HF are left open for a next question. Indicate the following in this scheme:
   i) whether the energy levels belong to H or F;
   ii) the names of the atomic orbitals (i.e. 1s, 2s, etc.);
   iii) for each electron use a cross (×) to indicate in which atomic orbital the electrons are in the ground state.

b) Why are the energy levels of one of the two atoms lower when compared to the energy levels of the other atom?

c) Which of the atomic orbitals contribute most to the groundstate of HF? Explain your answer.

d) Consider the following two molecular orbitals:
   \[ \psi_1 = 0.19(1s_H) + 0.98(2p_{z,F}) \]
   \[ \psi_2 = 0.98(1s_H) - 0.19(2p_{z,F}) \]

   Use the scheme of part a) to indicate where the energy levels corresponding to the orbitals \( \psi_1 \) and \( \psi_2 \) approximately will lie. Explain your choice. Note: the internuclear axis is oriented along the z-axis, the F-atom is placed in the origin and the H-atom on the positive z-axis.
Question 2. A classical particle with energy $E$ is moving in the potential represented in the figure on the left. The particle can only be found between the points $a$ and $b$ (due to energy conservation). An impenetrable “wall” is located at $x = a$. At $x = b$ the total energy $E$ equals the potential energy $V(x)$.

Which of the classical probability distributions $\rho(x)$, depicted on the right, best represents this situation? Recall that the probability of finding the particle in the interval $(x, x + dx)$ is given by $P(x, x + dx) = \rho(x)dx$.

(a) I
(b) II
(c) III
(d) IV
(e) V

↓ Explain your answer in 1-2 sentences in the space below. ↓

↓ Circle the statement below which describes how you feel about your answer. ↓

very certain  somewhat certain  somewhat uncertain  very uncertain
Question 3. The above graph shows a wave function \( \psi(x) \), plotted against \( x \). The probability to find the particle in region I, for example, is denoted by \( P(I) \). Order the probabilities of finding the particle in one of the regions I, II, or III, from largest to smallest.

(a) \( P(III) > P(I) > P(II) \)
(b) \( P(II) > P(I) > P(III) \)
(c) \( P(III) > P(II) > P(I) \)
(d) \( P(I) > P(II) > P(III) \)
(e) \( P(II) > P(III) > P(I) \)

\[ \downarrow \] Explain your answer in 1-2 sentences in the space below. \[ \downarrow \]

Question 4. The graph above shows a (rather artificial) wave function \( \psi(x) \), plotted against the location \( x \), over the range \((-2a, +4a)\). The wave function is equal to zero for all other values of \( x \). What is the probability to find the particle in the range \( 2a < x < 3a \) upon measurement?

(a) \( \frac{2}{9} \)
(b) \( \frac{1}{6} \)
(c) \( \frac{1}{4} \)
(d) \( \frac{1}{2} \)
(e) \( \frac{1}{3} \)

\[ \downarrow \] Explain your answer in 1-2 sentences in the space below. \[ \downarrow \]
Question 5. A particle in an infinite well (where $V(x) = 0$ between impenetrable walls) is in the energy eigenstate corresponding to the probability density $|\psi(x)|^2$ versus $x$ shown above. The energy of this state is $E = 1.2 \text{ eV}$. What is the energy of the lowest possible allowed energy state in this well?

(a) 0.0 eV 
(b) 0.3 eV 
(c) 0.4 eV 
(d) 0.6 eV 
(e) 1.2 eV 

↓ Explain your answer in 1-2 sentences in the space below. ↓ 

Question 6. The two (identical) pictures in the center of the figure above show a one-dimensional potential $V(x)$ and the energy level $E$ (dashed) of the sixth excited state. The other four picture represent wave functions. Which of these wave functions best represent the sixth excited state? Recall that the lowest energy is conventionally called the ground state, the next higher level corresponds to the first excited state and so forth.

(a) I 
(b) II 
(c) III 
(d) IV 
(e) There is something inconsistent about each one, so that none of them is an acceptable wave function for this state. 

↓ Explain your answer in 1-2 sentences in the space below. ↓ 

↓ Circle the statement below which describes how you feel about your answer. ↓
Chapter 9. Retention of Quantum Mechanical Concepts

Answers

The numbers between brackets denote the points assigned for a correct answer. For questions 2–7 one point is assigned for each correct answer.

Q 1 a) i. (1) The energy levels belong to H and F respectively.

ii. (1) Atomic orbitals for H: 1s, atomic orbitals for F: 1s, 2s, 2p

iii. (1) Configuration H: 1s

   1

   (one cross). Configuration F: 1s

   2

   2s

   2

   2p

   5

   (nine crosses).

b) (1) The energy levels of F are lower than that of H, because F has a higher nuclear electronic charge. The nucleus attracts the electrons stronger, or in other words: the potential energy of the electrons in the F atom is lower.

c) (1) As a rule of thumb: atomic orbitals that have approximately the same energy, mix best in molecular orbitals.

(1) Thus: the 1s of H and the 2p of F. The energy of a molecular orbital will become higher when atomic orbitals are mixed with higher energies. For the ground state, it is not logical to mix atomic orbitals that differ significantly in their energies.

d) (1) \( \psi_1 \) lies below \( 2p_z, F \), \( \psi_2 \) lies above \( 1s, H \)

(1) The \( \psi_1 \) and \( \psi_2 \) are superpositions of the atomic orbitals \( 1s_H \) and \( 2p_z, F \). Therefore, their energy level is near that of these two atomic orbitals. One will lie lower, the other higher. (Note: in this question no points are subtracted when the order of the orbitals is interchanged.)

e) (1) The energy of the orbitals \( \psi_1, \psi_2 \) is calculated through the expectation value:

(1) \[ \langle E_{1,2} \rangle = \int \psi_{1,2}^* \hat{H}_{HF} \psi_{1,2} d\tau \]

e) (1) The following sketch should be drawn:

\[ \psi_1 \quad \psi_2 \]

(1) As the orbital \( \psi_1 \) has a high value between the two nuclei, \( |\psi_1|^2 \) will also have a high value. This means that the probability of finding the electron between the two nuclei is large. This results in bonding. Stated differently: the curvature of the orbital \( \psi_1 \) is smaller than that of \( \psi_2 \) (there is one node less). This causes a lower energy for the \( \psi_1 \) orbital.

Q 2 e

Q 3 e

Q 4 a

Q 5 b

Q 6 d

Q 7 c
Question 1: Box with a step

In the course Quantum Physics I we have considered the infinite square well (a “box”) and the potential up-step. Both have exact solutions. In this problem we will look at a combination of the two: a box with a step. This problem does not have an exact/analytic solution. We want to find the energy eigenvalues of this problem.

The time independent Schrödinger equation is:

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x).\]

Given the following potential (see the figure):

\[V(x) = \begin{cases} V_0 > 0 & \text{for } -a < x < 0, \\ 0 & \text{for } 0 < x < a, \\ \infty & \text{elsewhere}. \end{cases}\]

In this problem we will look at the situation for which \(E > V_0\). In this case, the solution to the Schrödinger equation is:

\[\psi_L = A \sin qx + B \cos qx \quad \text{for } -a < x < 0,\]

\[\psi_R = C \sin kx + D \cos kx \quad \text{for } 0 < x < a.\]

a) For what values of \(q\) and \(k\) is the given wave function a solution to the Schrödinger equation?

b) What boundary conditions must hold at \(x = -a\) and \(x = a\)? Explain why these boundary conditions must hold.

What two equations follow when we impose these boundary conditions?

c) What are the continuity conditions that hold at \(x = 0\)? Use these conditions to express \(C\) in \(A\) and \(D\) in \(B\).
When the expressions found for $C$ and $D$ are used in the equations that follow from the boundary conditions in b), we find the following equation (you do not have to show this):

$$\sqrt{1 - \left(\frac{z_0}{z}\right)^2} = -\frac{\tan \sqrt{z^2 - z_0^2}}{\tan z},$$

Where we have defined: $z \equiv k\alpha$, $z_0 \equiv \frac{\pi}{k\alpha}$ and so: $q_0 = z^2 - z_0^2$.

We cannot solve this equation analytically. In Figure 1 the two functions are plotted, where we have chosen $z_0 = \pi$.

Figure 1: Plot of $\sqrt{1 - \left(\frac{z_0}{z}\right)^2}$ (solid) and $-\frac{\tan \sqrt{z^2 - z_0^2}}{\tan z}$ (dashed) for $z_0 = \pi$ and $z_0 < z < 3z_0$.

(The vertical lines are asymptotes.)

Question 2. The above graph shows a wave function $\psi(x)$, plotted against $x$. The probability to find the particle in region I for example, is denoted by $P(I)$. Order the probabilities of finding the particle in one of the regions I, II, or III, from largest to smallest.

(a) $P(III) > P(I) > P(II)$
(b) $P(II) > P(I) > P(III)$
(c) $P(III) > P(II) > P(I)$
(d) $P(I) > P(II) > P(III)$
(e) $P(II) > P(III) > P(I)$

Explain your answer in 1-2 sentences in the space below.

Circle the statement below which describes how you feel about your answer.

<table>
<thead>
<tr>
<th>very certain</th>
<th>somewhat certain</th>
<th>somewhat uncertain</th>
<th>very uncertain</th>
</tr>
</thead>
</table>

d) Argue that from the numerical solution of the above equation it follows that the system is quantized.

e) How many energy eigenvalues does this system have for the situation that $E > V_0$?
f) What energy does the state have with the lowest possible energy? In your answer you can use $m$, $\hbar$ and $a$.

g) The boundary, and continuity conditions together give four equations. In total however, we have five unknowns: $A, B, C, D$ and the energy $E$. What condition can you think of to fix all five unknowns? Explain what the meaning of this condition is.
Question 3. The graph above shows a (rather artificial) wave function $\psi(x)$, plotted against the location $x$, over the range $(-2a, +4a)$. The wave function is equal to zero for all other values of $x$. What is the probability to find the particle in the range $2a < x < 3a$ upon measurement?

(a) $2/9$
(b) $1/6$
(c) $1/4$
(d) $1/2$
(e) $1/3$

↓ Explain your answer in 1-2 sentences in the space below. ↓

Question 4. The graph above shows a (rather artificial) wave function $\psi(x)$, plotted against $x$, given by the two "spikes" shown, each of width $\Delta a$. The wave function is zero for all other values of $x$. Which of the expressions below is closest to the value of the spread or uncertainty in the position variable, namely $\Delta x$. Recall that

$$\Delta x \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2},$$

where $\langle \ldots \rangle$ denotes average, or expectation value.

(a) $\Delta x = 3a/5$
(b) $\Delta x = 2a$
(c) $\Delta x = 2\Delta a$
(d) $\Delta x = 4a/5$
(e) $\Delta x = \Delta a$

↓ Explain your answer in 1-2 sentences in the space below. ↓

↓ Circle the statement below which describes how you feel about your answer. ↓
Question 5. The figure on the left indicates a particle of energy $E$ near the boundary of a "step up, then down" potential located between $x = a$ and $x = b$, with $0 < E < V_0$. If you solve the time-independent Schrödinger equation in the region $(a,b)$ using this potential and this energy, which of the possible wave functions on the right could you find?

(a) I and II only,
(b) III only,
(c) I only,
(d) I and III only,
(e) I, II, and III are all possible.

$\downarrow$ Explain your answer in 1-2 sentences in the space below. $\downarrow$

Question 6. A particle in an infinite well (where $V(x) = 0$ between impenetrable walls) is in the energy eigenstate corresponding to the probability density $|\psi(x)|^2$ versus $x$ shown above. The energy of this state is $E = 1.2$ eV. What is the energy of the lowest possible allowed energy state in this well?

(a) 0.0 eV
(b) 0.3 eV
(c) 0.4 eV
(d) 0.6 eV
(e) 1.2 eV

$\downarrow$ Explain your answer in 1-2 sentences in the space below. $\downarrow$
Question 7. A particle of energy $E$ is incident, from the left, on a step potential of height $V_0 < E$ as shown in the figure above on the left. This problem is often analyzed using plane-wave solutions consisting of incident (I), reflected (R) and transmitted (T) components. The solution to the time-independent Schrödinger equation is given by:

$$\psi(x) = \begin{cases} I e^{ikx} + Re^{-ikx} & \text{for } x \leq 0 \\ T e^{iqx} & \text{for } x \geq 0 \end{cases}$$

where $k = \sqrt{2mE/\hbar^2}$ and $q = \sqrt{2m(E-V_0)/\hbar^2}$.

Which of the waveforms, shown in the figures I, II, III, IV, and V, best represents the true solution in this problem? Note that in the figures only the real part of $\psi(x)$ is represented.

(a) I, (b) II, (c) III, (d) IV, (e) V.

Explain your answer in 1-2 sentences in the space below.

(1) Which of the waveforms, shown in the figures I, II, III, IV, and V, best represents the true solution in this problem? Note that in the figures only the real part of $\psi(x)$ is represented.

(a) I, (b) II, (c) III, (d) IV, (e) V.

Explain your answer in 1-2 sentences in the space below.

(1) $q = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

(1) $k = \frac{\sqrt{2mE}}{\hbar}$

b) $\psi_L(-a) = 0$ and $\psi_R(a) = 0$

(1) These boundary conditions are imposed because on the boundary $V \to \infty$ and $\psi$ can only be a solution if it equals zero.

The following two equations follow from the above boundary conditions:

$$\begin{align*}
- A \sin qa + B \cos qa &= 0 \\
C \sin ka + D \cos ka &= 0
\end{align*}$$

(1) On $x = 0$ we have the following continuity conditions:

$$\begin{align*}
\psi_L(0) &= \psi_R(0), \\
\psi'_L(0) &= \psi'_R(0).
\end{align*}$$

From this it follows:

$$\begin{align*}
(1) \quad C &= \frac{q}{k} A, \\
(1) \quad D &= B.
\end{align*}$$

d) (1) The solutions are given by the intersections in the graph. Thus, there are discrete values for $z$ and hence discrete values for $E$. The system is thus quantized.

e) (1) There are infinitely many solutions, because $E > V_0$ and hence $z > z_0$. In that region there are infinitely many intersections.

f) (1) The intersection with the smallest value of $z$ is $z_{\text{min}} \approx 4.05$.

(1) Because $z = ka = a\sqrt{2mE/\hbar^2}$, we have $E_{\text{min}} = \frac{1}{2m} \left( \frac{2m}{a^2} \right)^2 \approx \frac{\hbar^2}{2m} \left( \frac{a}{\hbar} \right)^2$. 

Question 2 e

Question 3 a

Question 4 d

Question 5 a

Question 6 b

Question 7 d
References


