Assessment of Quantum Mechanical Concepts

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Abstract

Detroit Mercy offers a comprehensive engineering program with degrees in mechanical, civil, robotics and mechatronic systems, electrical, computer, environmental, and architectural engineering. The College of Engineering & Science has a well-established co-operative education program with a long history of placing graduates into the workforce upon graduation. Located in the city of Detroit the college has close ties to the automobile industry, its numerous suppliers and local defense contractors.

Detroit Mercy engineering students take a comprehensive physics sequence during the winter semester of their freshman year and fall semester of their sophomore year. The college offers PHY 3690 Modern Physics with Device Applications as a junior level physics course. The course is required of electrical engineers and offered as an elective to other engineering students. The class covers introductory topics in quantum mechanics leading to a basic understanding of the behavior of charge carriers in solids. A description of the course and the students will be presented later in the paper. Students are introduced to entanglement and quantum computation with computer simulations of quantum measurements. We believe that a brief introduction to these topics helps students understand the relationship between operators and the results of a measurement of the wavefunction.

Over the past several years we have assessed students in the course with the Quantum Mechanics Conceptual Survey (QMCS).[1] This instrument was designed to be used as a general survey of students' conceptual understanding. One of the interesting aspects of this instrument is that engineering students in modern physics courses were considered during its development and validation. In this paper we will analyze our students' conceptual understanding of quantum mechanical concepts and compare them with those students that participated in the development of the survey. Responses to sample questions will be examined and student difficulties will be identified. We believe readers will be surprised as to how persistent certain student misconceptions appear to be.

Course Description and Content

Modern Physics with Device Applications PHY 3690 is a junior level course offered by the physics department. The class is required for electrical engineers and is a technical elective for other engineering or science majors—registration of non-electrical engineers is unusual. The class is offered in the winter term and for the past three years, the period over which the QMCS instrument was administered, the enrollment averaged 8 students per term; typically, one of those students was female. The prerequisite for the course is successful completion of one year of calculus-based general physics with the associated laboratories. The typical student has completed a course in differential equations with linear algebra. Engineering students are introduced to MATLAB [2] during their freshman year. We leverage this knowledge of the MATLAB environment along with their experience with linear algebra to manipulate vectors and matrices—the original language of quantum mechanics. The specific learning outcomes from the most recent syllabus are:

> Students will use distribution functions to describe physical systems and apply the concepts to blackbody radiation. They will analyze electromagnetic radiation in terms of the wave and particle models, and solve problems dealing with spontaneous and stimulated emission of radiation. Students will solve nonlinear equations using numerical techniques. They will apply the Bohr model to analyze electron energy levels in atoms and relate those levels to observed line spectra. Students will apply the de Broglie and Heisenberg hypotheses; analyze wave packets and recognize the probabilistic interpretation of the wave function. Students will use Dirac notation to represent quantum states and unitary matrices to represent operators. They will simulate quantum computation experiments utilizing MATLAB. Students will solve the Schrödinger equation in one dimension for various potentials. Students will identify cubic crystal lattices and use standard notation to identify planes and directions. They will identify dopant and impurity types; draw energy band diagrams and relate the structure of the bands to physical properties; develop the concepts of electrons and holes in materials and study the effects of their concentrations on space-charge and diffusion. They will analyze the statistics of electron occupation using Fermi-Dirac statistics; identify and analyze current flow mechanisms in pn junction diodes, solar cells, and transistors. Students will analyze nanoscopic materials such as graphene and other interesting 2-dimensional materials.

The course topics include:

1) Properties of Light
    a) Spectral Irradiance and Blackbody Radiation
    b) Photoelectric Effect and the Photon Concept
2) Nuclear Atom
    a) Atomic Spectra and the Rutherford-Bohr Model of Atomic Structure
    b) Spontaneous and Stimulated Emission of Radiation
3) Wave Properties of Matter
    a) The de Broglie Hypothesis and the Heisenberg Uncertainty Principle
    b) Wave Packets
4) Quantum Computation and Simulation
    a) Dirac Notation
    b) Matrices and Operators
    c) Mermin’s Device and Entanglement
5) The Schrödinger Equation
    a) One Dimensional Examples
    b) Expectation Values and Operators
    c) Quantum States and Superposition
6) Crystal Properties
    a) Hard Sphere Model and Density
    b) Crystal Lattices and Miller Notation
7) Quantum Theory of the Solid State
    a) Energy-Band Theory
    b) Quantum Statistical Mechanics
8) Charge carriers
    a) Donors and Acceptors
    b) Chemical Potential and Fermi Energy
    c) Drift and Diffusion Currents
9) Semiconductor Junctions
    a) Equilibrium Conditions
    b) Current-Voltage Characteristics
    c) Metal-Insulator-Semiconductor structures
10) Solar Cells and Lasers
    a) Optical Absorption and Gain
    b) Current-Voltage Characteristics
11) Nanoscopic Materials
    a) Graphene
    b) 2–dimensional electronic systems

The Dirac notation [3], [4] and curriculum associated with simulated quantum computation [5] are treated throughout the course. Mermin's Device [6] is discussed in the third week of class to introduce entanglement. After the publication of Mermin's original paper in 1981 he developed other variants of his device [7], [8] that are not discussed in the class. The other thought experiments that Mermin subsequently developed are more appropriate for an advanced audience; the devices he describes do not require perfectly correlated particles. The concept of entanglement is fundamental to quantum mechanics and was first introduced by Schrödinger in 1935. However, as Schroeder [9] points out, the word has been virtually absent from publication until the 1980's. Various aspects of quantum computation are revisited throughout the course as MATLAB projects. These projects escalate in complexity and are used to reinforce the value of the quantum simulations. The quantum computational simulations are based on the published work of Candela.[10]

Assessment Instrument

The QMCS 2.0 is a research-based instrument developed to survey students' conceptual understanding of quantum mechanics. It is a 12-question multiple choice survey of student understanding of various topics in introductory quantum mechanics or modern physics courses. As discussed by the authors, it is written using everyday language, it is conceptual in nature with no need to memorize formulas, the distractors are believed to be effective at discriminating students' preconceived notions, and most faculty believe that it is too easy. It is administered during the last week of the course and does not count against a student's grade. Part of the validation of the survey involved interviewing faculty that have recently taught a modern physics or quantum mechanics course. Faculty buy-in is believed to be an important factor that can affect teaching practice. Faculty have absolutely no consensus about which topics are important in a quantum mechanics course. Some believe that concepts should be taught while others are of the mindset of "shut up and calculate." The concepts that had the most overlap among faculty, listed from highest to lowest, were:

i. wave function and probability,
ii. wave-particle duality,
iii. Schrödinger equation,
iv. quantization of states,
v. uncertainty principle,
vi. superposition,
vii. operators and observables,
viii. tunneling,
ix. measurement.

Reviews of textbooks and syllabi showed a great deal of overlap in the topics covered and a surprising lack of discussion of measurement, wave function collapse etc.

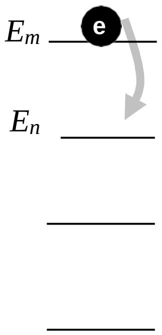
Our intent is to compare student responses from the published QMCS data to that of the students taking PHY 3690. The authors of the QMCS used input from faculty teaching modern physics for engineers in the design of the instrument so utilizing the instrument for our engineering students seems appropriate. To protect the fidelity of the QMCS we will not reproduce the test here. We do discuss some of the questions that were presented in the original manuscript. The QMCS authors recommend using the instrument as a formative assessment of student understanding of quantum mechanical concepts. The authors encourage faculty to administer the test in modern physics courses to inform their teaching and to publish results for the benefit of the broader community.

Sample Questions from Quantum Mechanics Conceptual Survey

Question 1 from the survey is shown below along with the percentage of responses from the QMCS group and from the modern physics courses at Detroit Mercy in Figure 1. The correct answer is given as selection D. Consider the distractors used for the problem. Clearly the problem is soliciting whether a student can recognize that the larger the energy difference between the electronic energy levels the larger the energy of the emitted photon and the greater the frequency (the shorter the wavelength) of the light.

Question 1

The diagram at right shows the electronic energy levels in an atom with an electron at energy level E_m. When this electron moves from energy level E_m to E_n, light is emitted. The greater the energy difference between the electronic energy levels E_m and E_n…



A. …the more photons emitted.
B. …the brighter (higher intensity) the light emitted.
C. …the longer the wavelength (the more red) of the light emitted.
D. …the shorter the wavelength (the more blue) of the light emitted.
E. More than one of the above answers is correct.

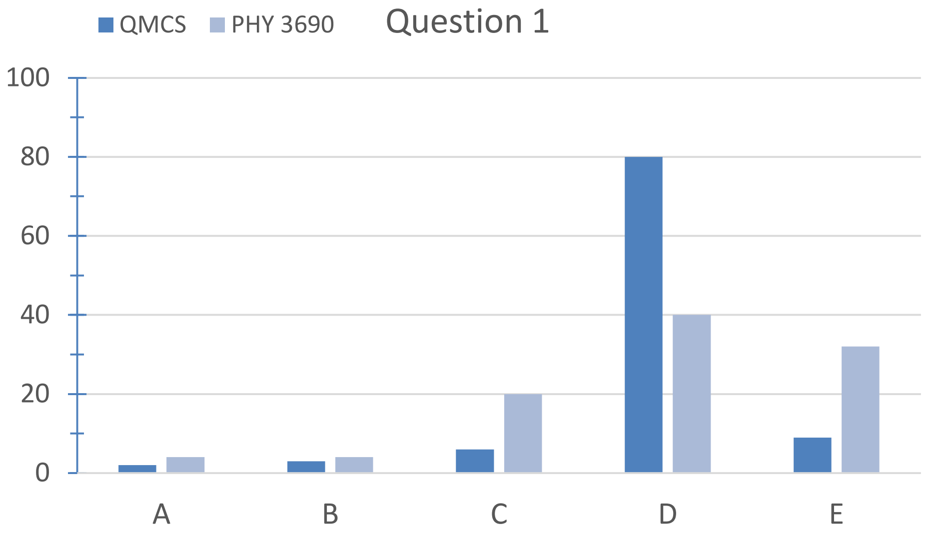


Fig. 1
Comparison of student responses from PHY 3690 with those from the QMCS to question 1. The authors indicate that the correct answer is D.

The distractor A indicates “more photons are emitted” which would refer to the transition rate between the two states – a topic for an advanced course. Response B states that “the brighter (higher intensity) the light emitted.” This response unfortunately can cause notable confusion. Brightness is related to intensity but requires the response of the human eye. The intensity has units of power per unit area and for a flux of monochromatic photons is equal to the energy per photon times the photon flux. If the transition rates are assumed to be independent of the energy difference then the greater the energy difference between the electron states, the greater the energy of the photon and hence the greater the intensity of the light. It can be argued that while response D is correct, response B is too and therefore the best response would be E. When the student responses are examined we note that 80% of QMCS students answered D while half as many of our students responded that way. If we look at the percent of students that answered D or E we see that 89% of QMCS students and 72% of our students answered that way.

Question 4 of the QMCS 2.0 is simple and perplexing. The question is shown below along with student responses in Figure 2. The authors argue that this question is difficult not because of students’ misconceptions but due to instruction. While validating the instrument they administered an assessment with this question in a pre- and post-test fashion.

Question 4

True or False: In the absence of external forces, electrons move along sinusoidal paths.
a. True
b. False

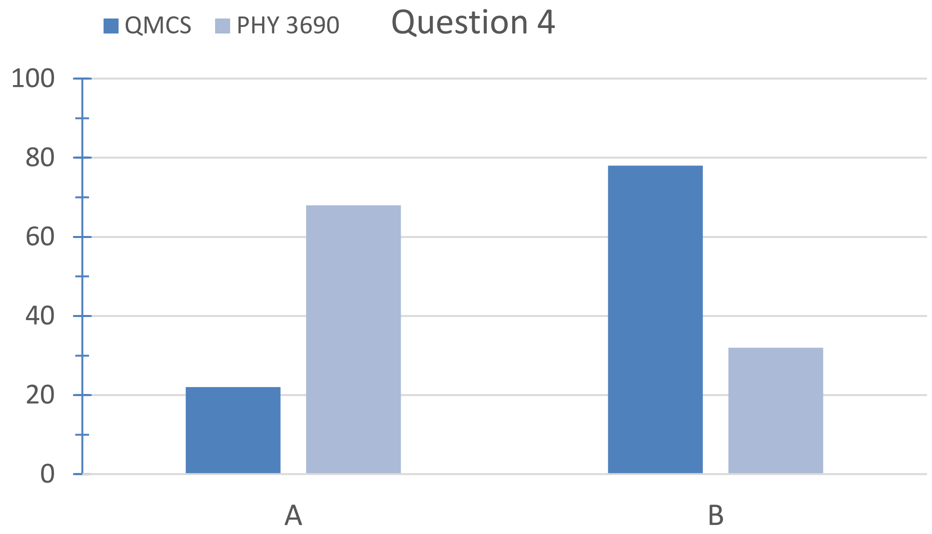


Fig. 2
Comparison of student responses from PHY 3690 with those from the QMCS to question 4. The authors indicate that the correct answer is B.

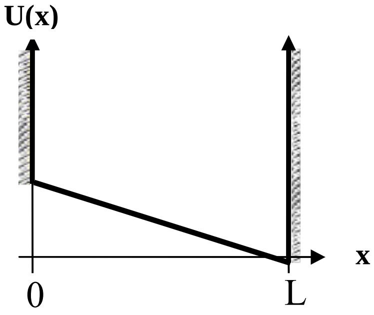
This was the only question where students did worse, often much worse, after instruction. They found that advanced undergraduates, graduate students and faculty often pick the wrong answer for this question because the literal meaning of the question is so “nonsensical” that they mentally translate it to mean the wavefunction instead of the path. Students responded differently

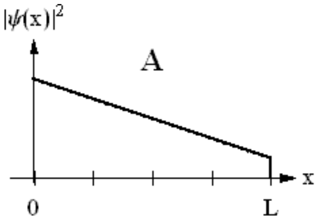
to this question if they were part of the modern physics cohort instead of the physics students in a quantum mechanics course. The interviews they conducted showed that the modern physics students almost never misinterpreted this question–path versus wavefunction. They considered the question at face value. McKagan, et. al. found that of the 46 students they interviewed only two thought it referred to the wavefunction and the rest, no matter how they responded, interpreted it as meaning the path of the electron was sinusoidal. They tried numerous variations in wording and have not found any question that worked better than the current version.
We have no clear understanding of why about 2/3 of Detroit Mercy students would respond that free electrons follow sinusoidal paths. It was found in class that the solution to the Schrödinger equation for an electron in the absence of an external force is of the form $\sin\left(kx-\omega t\right)$ or $e^{i(kx-\omega t)}$ nowhere were sinusoidal paths mentioned. The authors of the QMCS indicate that as a result of pre- and post-test administration of the QMCS the incorrect student responses to this question are a result of instruction. When they conducted student interviews several students said that when photons were discussed the instructor drew a wavy line on the board, etc.

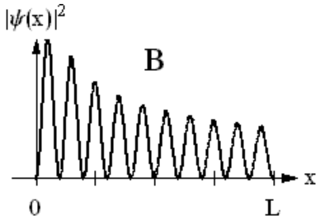
Question 10 of the QMCS 2.0 relates the shape of the wavefunction to the shape of the external potential. Here students need to recognize several important aspects of the wavefunction and potential energy. The total energy of the particle is constant so where the potential energy is greatest, the kinetic energy is the least. The kinetic energy is related to the speed and thus the wavelength of the particle.

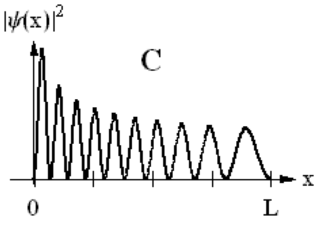
Question 10

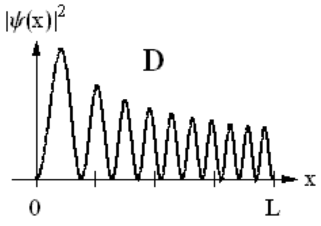
The figure at right shows a potential energy function $U(x)$, where the potential energy is infinite if x is less than 0 or greater than L, and has a slanted bottom in between 0 and L, so that the potential well is deeper on the right than on the left. Which of the plots of $|\psi(x)|^2$ vs. x is most likely to correspond to a stationary state of this potential well?











E. More than one of these is a possible stationary state.

Examination of the graph shows that the kinetic energy is greatest near the right-hand side of the well. If the kinetic energy is the greatest there, then the speed is the greatest. If the speed is the greatest, then it spends less time there. The amplitude should be greater at the left end, near $x = 0$, and the wavelength should be the smallest at the right end where $x = L$ so the correct response is D. The percentage of responses for the QMCS sample group and PHY 3690 are shown below in Figure 3. Only 27% of QMCS students responded correctly while 20% of PHY 3690 did. The distribution of responses shows that not many students believed in a linear wavefunction as being correct, but the distribution is close to that of random guessing. This is not surprising given the multistep reasoning required to determine the correct response.

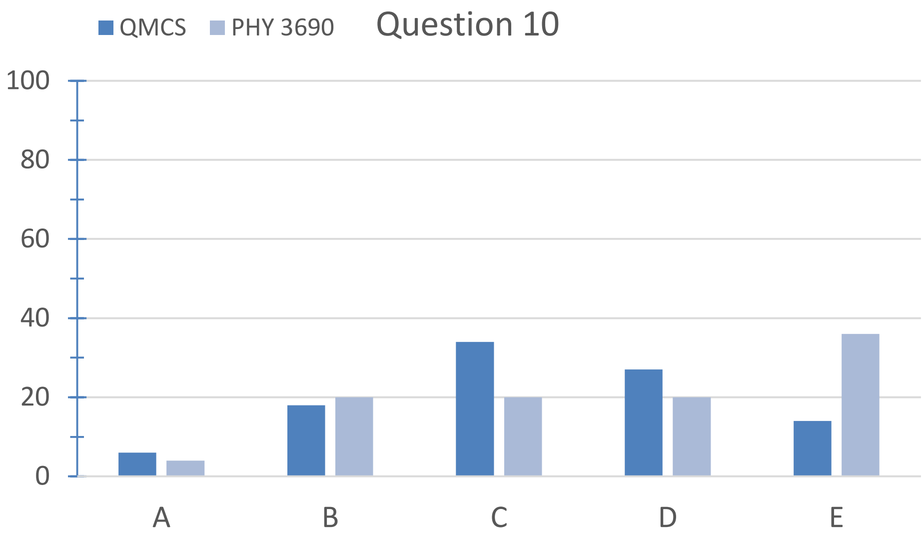


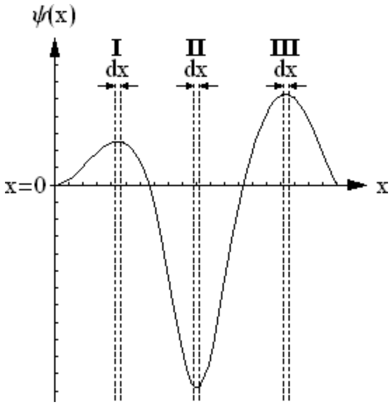
Fig. 3
Comparison of student responses from PHY 3690 with those from the QMCS to question 10. The authors indicate that the correct answer is D.

The authors of the QMCS designed Question 11 to measure student understanding of the relationship between the wavefunction and the probability density. The faculty members the authors surveyed indicated that it was an important topic and that it was also a good question. Over 90% of the QMCS students answered the question correctly while 72% of the PHY 3690 responded correctly. The reasonable way to answer this question is to look at either the absolute value of the wavefunction–the correct way–or to look at the value of the wavefunction. In the PHY 3690 sample, 16% of the students responded A.

Question 11

> The plot at right shows a snapshot of the spatial part of a one-dimensional wave function for a particle, $\psi(x)$, versus x. $\psi(x)$ is purely real. The labels, I, II, and III, indicate regions in which measurements of the position of the particle can be made. Order the probabilities, P, of finding the particle in regions I, II, and III, from biggest 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)



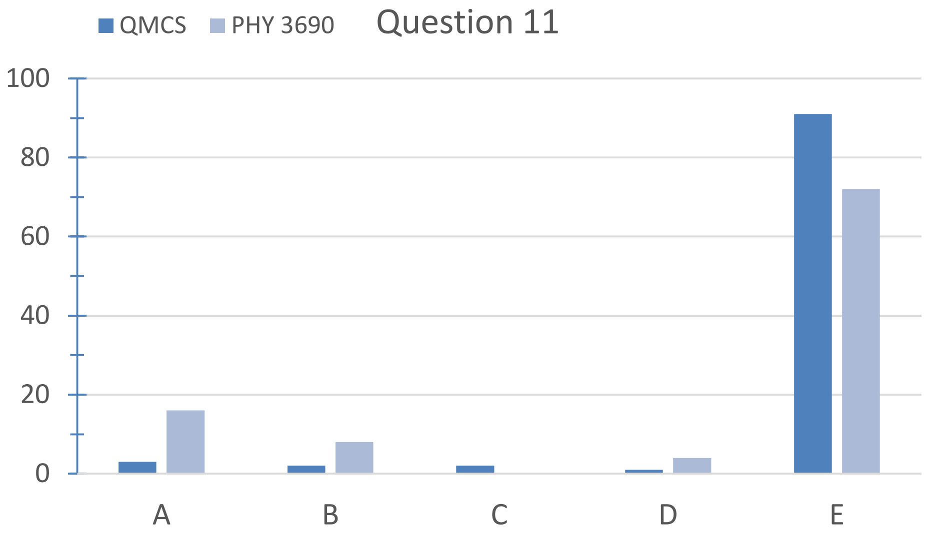
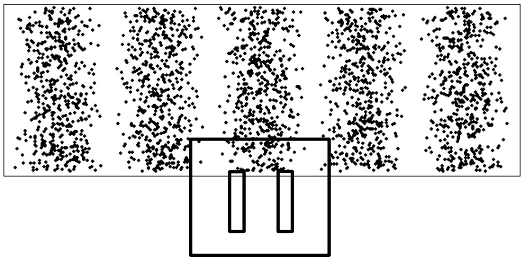


Fig. 4
Comparison of student responses from PHY 3690 with those from the QMCS to question 11. The authors indicate that the correct answer is E.

Wave-particle duality is a concept that was viewed by faculty as being very important. Question 12 of the assessment addresses this topic. Several versions of this question have been attempted and the authors have not found one that all physics professors agree is the best. The comparison of the QMCS cohort with the Detroit Mercy students is shown below in Figure 5.

Question 12

You shoot a beam of photons through a pair of slits at a screen. The beam is so weak that the photons arrive at the screen one at a time, but eventually they build up an interference pattern, as shown in the picture at right. What can you say about which slit any particular photon went through?



A. Each photon went through either the left slit or the right slit. If we had a good enough detector, we could determine which one without changing the interference pattern.
B. Each photon went through either the left slit or the right slit, but it is fundamentally impossible to determine which one.
C. Each photon went through both slits. If we had a good enough detector, we could measure a photon in both places at once.
D. Each photon went through both slits. If we had a good enough detector, we could measure a photon going through one slit or the other, but this would destroy the interference pattern.
E. It is impossible to determine whether the photon went through one slit or both.

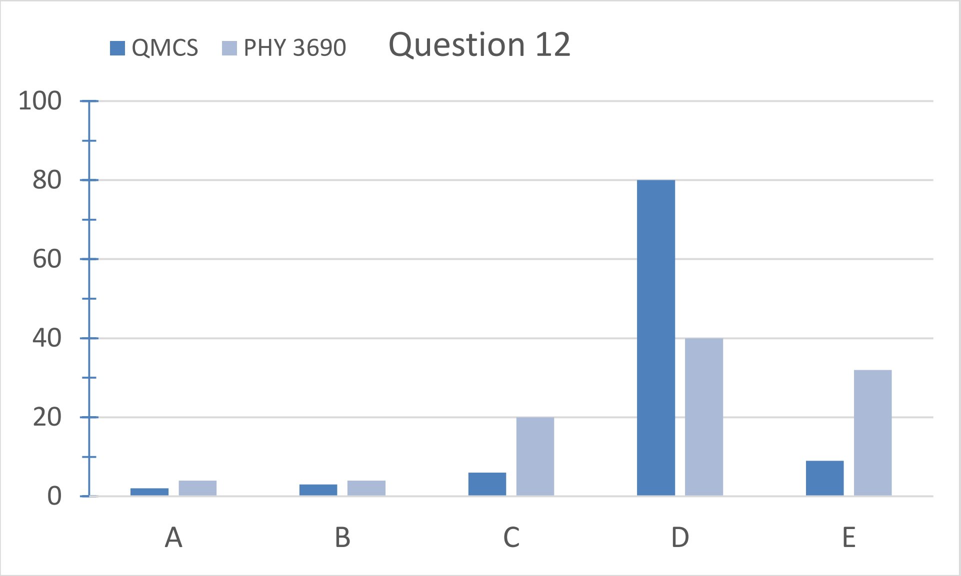


Fig. 5
Comparison of student responses from PHY 3690 with those from the QMCS to question 12. The authors indicate that the correct answer is D.

Statistical Analysis and Discussion

The Quantum Mechanics Conceptual Survey is a useful instrument to gauge student understanding of quantum mechanical concepts. The assessment should be considered difficult and care needs to be taken as to its proper use. It’s value as a formative rather than summative assessment is apparent. Shown below in Figure 6 is the percentage of students responding correctly, according to the authors, for the QMCS sample and the PHY 3690 cohort. The results for students responding at random are also shown.

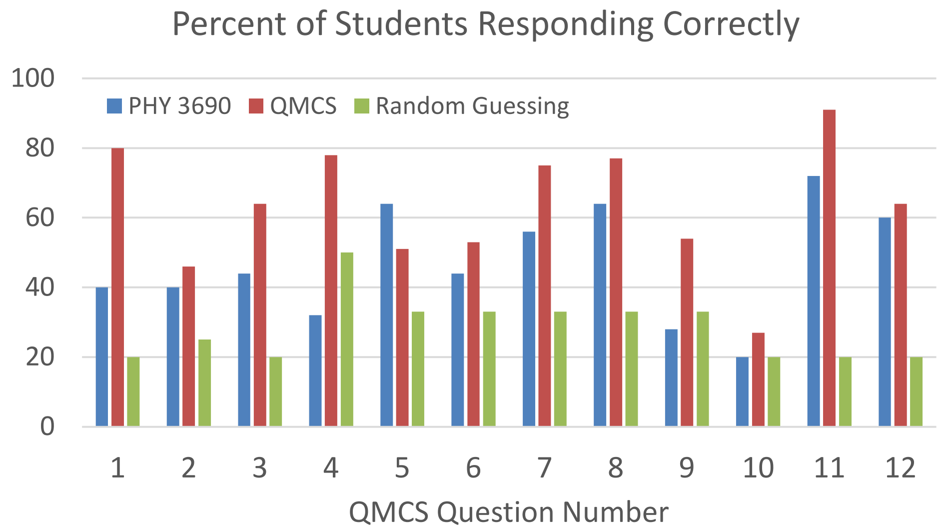


Fig. 6
Comparison of student responses from PHY 3690 with those from QMCS and the expected result from random guessing.

The Kuder–Richardson Formula 20 (KR-20) coefficient is a measure of the reliability of an assessment.[11], [12] For a test with K=12 items the KR-20 reliability coefficient, r, is given by

$$r = \frac{K}{K-1}\left[1 - \frac{\sum_{i=1}^{K} u_i w_i}{\sigma^2}\right]$$

where u_i is fraction of correct responses for the i^{th} question and w_i is the fraction of incorrect responses for the i^{th} question so $u_i + w_i = 1$. The variance, σ^2, is the square of the standard deviation. Table I shows the number of students, the mean, variance, standard deviation, median, and sum of the product of correct and incorrect responses for the students in the PHY 3690 course. The sum of the product of correct and incorrect responses if students chose all the answers at random is 2.3. If all students responded either correctly or incorrectly the sum would be zero and we would have r = 1.09. The maximum value of the sum is easy to see. Each term in the sum looks like $z(1-z)$, the maximum occurs when $\frac{d}{dz}z(1-z) = 0$, which corresponds to $z = 0.5$. If half of the students respond correctly, each of the twelve terms in the sum is 0.25 and the greatest value of 3.0 occurs. In Table I we summarize the results of the statistical analysis of the scores on the QMCS. The KR-20 reliability coefficient has a value of 0.47 which is low, typical values exceed 0.70. The authors report a Cronbach Alpha of 0.44 which is a similar measure to the KR-20 coefficient; and they argue that the low value is due to the fact that the QMCS measures multiple concepts that are independent of each other.

N	mean	variance	std. dev.	median	$\sum_{i=1}^{i=29} u_i w_i$	r
25	5.64	4.71	2.17	5	2.70	0.47

Table I
Table containing the number of students, mean, variance, standard deviation, median, and sum of the product of correct (u_i) and incorrect (w_i) responses, and the KR-20 reliability coefficient for students given the QMCS test.

In Figure 7 below, we show the distribution of student scores on the QMCS. The percent of students that score less than or equal to a given score is a cumulative distribution function (CDF). A Gaussian distribution is represented by $\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ where x is the score, μ is the mean and σ the standard deviation, σ^2 is the variance. For a Gaussian distribution the cumulative distribution function is given by $\frac{1}{2}\left(1+erf\left(\frac{(x-\mu)}{\sqrt{2}\sigma}\right)\right)$. The error function, *erf(x)*, is a standard function given by $\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2} dt$.

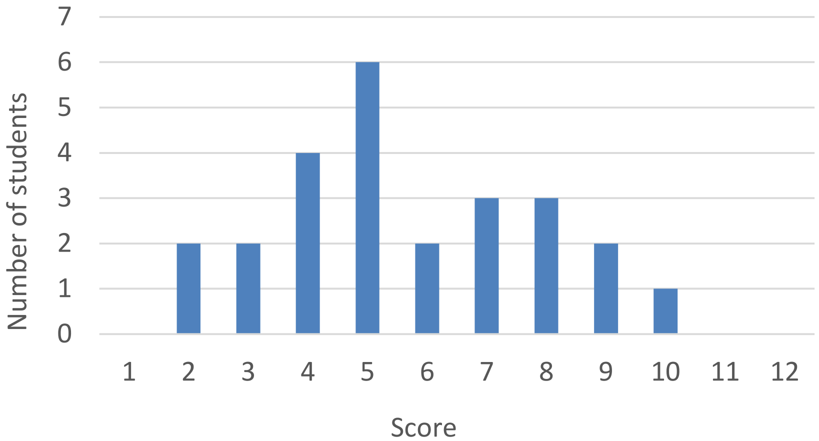


Fig. 7
Number of students from PHY 3690 with a given score for a sample $N = 25$.

In Figure 8 the cumulative distribution function for the PHY 3690 student scores is shown in normalized form, the total number of students tested was 25. The vertical axis is the fraction of those students that had a score less than or equal to the value on the horizontal axis. Also shown is the calculated CDF from the error function described above with the given mean and standard deviation. Additional testing of the CDF is shown below in Figure 9. In this figure we show the actual CDF plotted against the calculated CDF from the error function with the given mean and standard deviation.

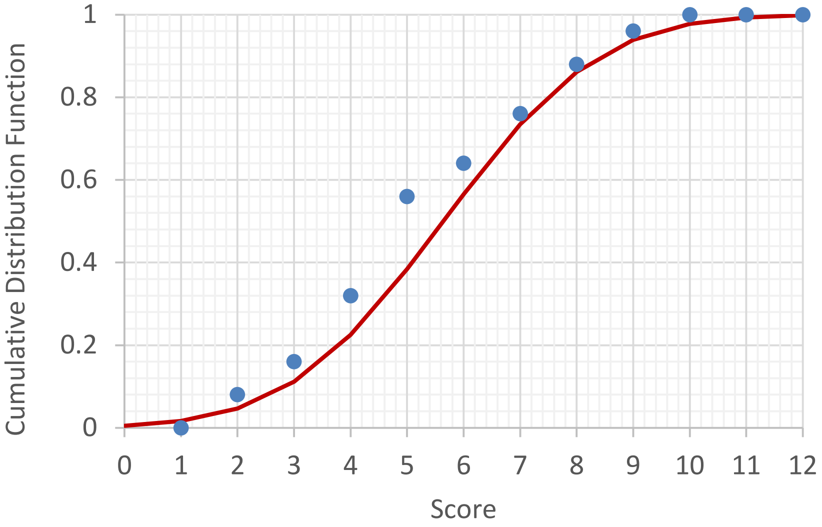


Fig. 8
Cumulative distribution function of scores for PHY 3690 students. The vertical axis is normalized to N=25, the total number of students. The solid blue circles represent the actual binned data while the red line is the error function with μ = 5.64 and σ = 2.17.

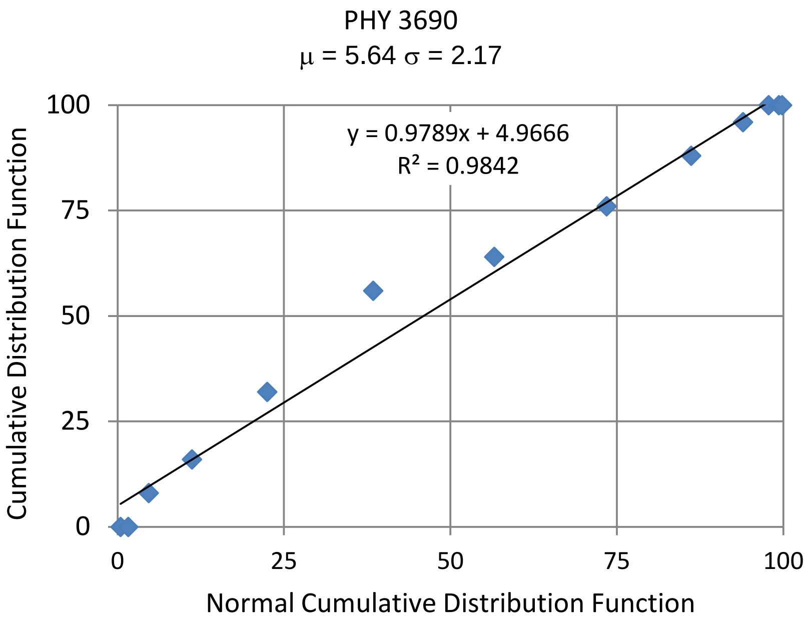


Fig. 9
Actual cumulative distribution functions for PHY 3690 (blue diamonds) versus calculated normal cumulative distribution function with the given mean and standard deviation. The least squares linear fit is included.

Below in Table II the percent of student responses to each question of the QMCS.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
A	4	20	8	68	12	24	12	4	44	4	16	20
B	4	4	4	**32**	**64**	**44**	**56**	**64**	28	20	8	16
C	20	**40**	12	0	24	32	32	32	**28**	20	0	4
D	**40**	36	**44**	0	0	0	0	0	0	**20**	4	**60**
E	32	0	32	0	0	0	0	0	0	36	**72**	0

Table II
Table containing the percentage of PHY 3690 student responses for each question on the QMCS.
The authors indicated correct responses are shown in blue. *N*= 25.

Conclusion

The Quantum Mechanics Conceptual Survey is a useful tool to assess student understanding of various concepts in quantum mechanics. The survey was developed, in part, by considering engineering students in a modern physics course. We believe that the instrument should be used as a formative assessment to influence instruction and pedagogy and its use as a summative instrument should be avoided at all costs—the authors of the survey agree with this conclusion.

Below in Figure 10 we show the percentage of correct student responses as a function of the final grade that the student received in the course. Detroit Mercy uses a 4-point grading scale for calculating grade point averages. In addition, students are given + and – grades according to the following scheme: A = 4.00, A– = 3.67, B+ = 3.33, B = 3.00, etc.

Examination of Figure 10 makes it apparent that there is not a strong correlation between the final grade that a student earned and the performance on the QMCS. This is, of course, due to a variety of factors. One being that basic topics in quantum mechanics constitute only a relatively small fraction of the topics covered in a modern physics for engineers.

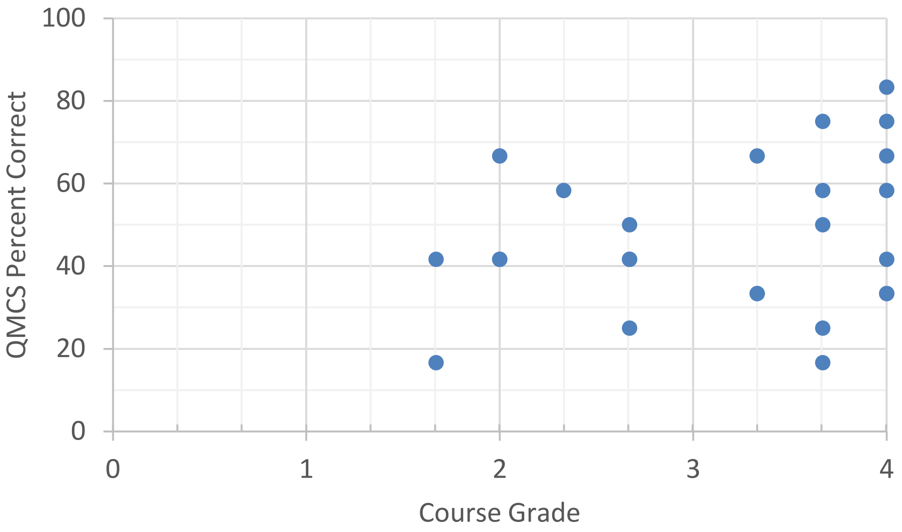


Fig. 10
Relationship between percent correct on QMCS and final grade in PHY 3690. At Detroit Mercy students #receive letter grades corresponding to a grade point average A = 4.00, A- = 3.67, B+ = 3.33, etc.

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