

جامعة : المنصورة

كلية : العلوم

قسم / الكيمياء

توصيف مقرر دراسي

١ - بيانات المقرر		
الرمز الكود : ك ٤ ٤ ٢	اسم المقرر : Quantum chemistry	المستوى : الثاني
البرنامج : الكيمياء	عدد الوحدات الدراسية : ٢ نظري : ٢ تمارين : ١ عملي : -	

٢ - هدف المقرر : For students undertaking this course, the aims are to: 1 - Introduce the basic concepts of quantum mechanics. 2 - Acquire the students skills to grasp challenging concepts of equations of motion of particles 3 - Outline the basic information of the world applications of the quantum mechanics. 4 - Enable the students to solve problems and obtain the energy levels and eigen functions of particles quantum mechanically by using Schrödinger equation	
٣ - المستهدف من التدريس المقرر :	
a- Knowledge and Understanding : a - 1 - Explain the basic concept and the origin of quantum mechanics a - 2 - Acquire an understanding of more knowledge in physical quantities describing any particle. a - 3 - Know the concepts of Schrödinger Eq. and its applicable problems a - 4 - Recognize the different behavior quantum mechanical particles. On completing this course, students will be able to:	أ-المعلومات والمفاهيم:
b- Intellectual Skills: On completing this course, students will be able to:	ب-المهارات الذهنية

<p>b - 1 - Distinguish between the concept of quantum mechanics and classical mechanics</p> <p>b - 2 - Apply mathematical formula of Schrödinger equation in solving challenging problems</p> <p>b - 3 - Analyze and solve the different problems in quantum mechanics.</p>	
<p>c-Professional and Practical Skills: On completing this course,</p> <p>c - 1 - Choose and classify data for obtaining the Schrödinger Eq.</p> <p>c - 2 - Apply and solve the equation of motion of a mechanical system quantum mechanically.</p> <p>c - 3 - Compare between quantum and classical principles to overcome the problems appear in classical mechanics.</p> <p>students will be able to:</p>	<p>ج- المهارات المهنية الخاصة بالمقرر:</p>
<p>d-General and Transferable Skills: On completing this course,</p> <p>d - 1 - Solve problems describing different quantum mechanical systems via simulation method.</p> <p>d - 2-Collect and analyze the data to find the solutions of the constructed equations of motion.</p> <p>d - 3- Present short reports in oral and written means on some specified subjects.</p> <p>☐ d - 4- Work effectively both in a team, and independently to obtain the data required to overcome the quantum mechanical problems</p> <p>students will be able to:</p>	<p>د- المهارات العامة :</p>
<p>Ch. 1: Introduction Postulates of Q. M., Schrödinger Eq. in space and momentum coordinates</p> <p>Ch. 2: One-dimensional systems 2.1:-Bound states: infinite, finite, SHO, Morse and Delta function potentials. Linear infinite potential using momentum space. Operating method to solve SHO potential. 2.2:-Unbound states: Free particle, potential step, tunneling effect and radioactive alpha decay- periodic potential.</p> <p>Ch. 3: Three-dimensional systems 3.1:-Rectangular Coordinates: three-dimensional box, three-dimensional harmonic oscillator and the degeneracy of their energy levels.3.2:- Cylindrical Coordinates: three-dimensional harmonic</p>	<p>٤- محتوى المقرر:</p>

<p>oscillator.3.3:- Spherical Coordinates: spherical-symmetric potential-isotropic harmonic oscillator-the space rotator-the Hydrogen-like atoms.</p> <p>Ch. 4: Angular momentum operators Basic properties, Cartesian and spherical components, commutates relations, eigen values and eigen functions of the angular momentum operators, eigen values and eigen functions of the ladder operators.</p> <p>Ch. 5: Approximation methods Time-independent perturbation theory for nondegenerate state (anharmonic oscillator and electric field perturbations).Time-independent perturbation theory for degenerate state (Stark effect in hydrogen atoms).</p>												
<p>4.1 - Lectures using data show and board.</p> <p>4.2 - Discussion sessions</p> <p>4.3 - Problem classes</p> <p>4.4 - class activity</p>			٥- أساليب التعليم والتعلم:									
<p>The same as normal students, only skeletal disabilities are allowed in the Faculty of Science.</p>			٦- أساليب التعليم والتعلم للطلاب ذوي القدرات المحدودة:									
٧- تقويم الطلاب :												
<p>7- Student Assessment Methods</p> <table><tr><td>Final exam</td><td>to assess</td><td>a1-a4, b1-b3 and c2, c3,d1</td></tr><tr><td>Oral exam</td><td>to assess</td><td>a1-a4, b1-b3</td></tr><tr><td>Mid-term exam</td><td>To assess</td><td>a1-a4, b1-b3 and c2, c3,d1</td></tr></table>			Final exam	to assess	a1-a4, b1-b3 and c2, c3,d1	Oral exam	to assess	a1-a4, b1-b3	Mid-term exam	To assess	a1-a4, b1-b3 and c2, c3,d1	أ- الأساليب المستخدمة :
Final exam	to assess	a1-a4, b1-b3 and c2, c3,d1										
Oral exam	to assess	a1-a4, b1-b3										
Mid-term exam	To assess	a1-a4, b1-b3 and c2, c3,d1										
<p>Assessment Schedule</p> <table><tr><td>Assessment 1</td><td>Week #final exam</td><td>Week 16</td></tr><tr><td>Assessment 2</td><td>Week #oral exam</td><td>Week 16</td></tr><tr><td>Assessment 3</td><td>Week #mid-term</td><td>Week 7</td></tr></table>			Assessment 1	Week #final exam	Week 16	Assessment 2	Week #oral exam	Week 16	Assessment 3	Week #mid-term	Week 7	ب- التوقيت :
Assessment 1	Week #final exam	Week 16										
Assessment 2	Week #oral exam	Week 16										
Assessment 3	Week #mid-term	Week 7										

	exam		
<i>Weighting of Assessments</i>			ج- توزيع الدرجات :
Final-Term Examination	80%		
Oral Examination	10%		
Practical Examination	0%		
Semester work	0%		
Mid-term examination	10%		
Other types of assessment	0%		
Total	100%		
٨- قائمة الكتب الدراسية والمراجع :			
			أ- مذكرات:
1 - Theoretical Phys., V3 Quantum Mech., B. G. Levich,1973 2 - Advanced Quantum Theory, S.L Fields, Gupta,1Ed, 1982 3 - Quantum Chemistry, R.K. Prasad, New Delhi,2000			ب- كتب ملزمة
			ج- كتب مقترحة :
http://www.whfreeman.com/pchem7/ http://www.mpcfaculty.net/ron_rinehart/physchem.htm			د- دوريات علمية أو نشرات..

مصفوفة المعارف والمهارات المستهدفة من المقرر الدراسي

المحتويات للمقرر	اسبوع الدراسة	المعارف الرئيسية	مهارات ذهنية	مهارات مهنية	مهارات عامة
Ch. 1: Introduction Postulates of Q. M., Schrödinger Eq. in space and	1	a1,a2,a3	b1	c1	

momentum coordinates					
Ch. 2: One-dimensional systems 2.1:-Bound states: infinite, finite, SHO, Morse and Delta function potentials. Linear infinite potential using momentum space. Operating method to solve SHO potential. 2.2:- Unbound states: Free particle, potential step, tunneling effect and radioactive alpha decay- periodic potential.	2-4	a2,a3			
Ch. 3: Three-dimensional systems 3.1:-Rectangular Coordinates: three-dimensional box, three-dimensional harmonic oscillator and the degeneracy of their energy levels.3.2:- Cylindrical Coordinates: three-dimensional harmonic oscillator.3.3:- Spherical Coordinates: spherical-symmetric potential-isotropic harmonic oscillator-the space rotator-the Hydrogen-like atoms.	5-7	a3,a4	b2,b3		d1-d4
Ch. 4: Angular momentum operators Basic properties, Cartesian and spherical components, commutate relations, eigen values and eigen functions of the angular momentum operators, eigen values and eigen functions of the ladder operators.	8-10	a3,a4			
Ch. 5: Approximation methods Time-independent perturbation theory for nondegenerate state (anharmonic oscillator and electric field perturbations).Time-independent perturbation theory for degenerate state (Stark effect in hydrogen atoms).	11-12	a3,a4		c2,c3	d1-d4

أستاذ المادة : أ.د./أحمد محمد الجراحي عبد الحليم رئيس مجلس القسم العلمي : أ.د /سالم السيد
سمرة