Problem Set PS04

ISSUED: 2/7/02 **Due: 2/14/02**

Prof. Darin J. Ulness   Name ____________________

Instructions. Complete all questions before class on the due date. You are encouraged to work together. Be sure to struggle with the problem before seeking help. Many of the exercises are very similar to problems in the book. Understanding the solution to these problems will be helpful in completing the assigned exercises.

Mathematical Exercises

1. What is the result of operating on the following functions with the inversion operator: $\hat{\imath}f(x,y,z) = f(-x,-y,-z)$? Is the function an eigenfunction of the operator? If so, what is the eigenvalue? Label the function as gerade or ungerade when appropriate.

   (a) $f = \frac{x^2+y^2+z^4}{x+y+z}$

   (b) $f = xyz^2$

   (c) $f = xyz - z$

2. What is the result of operating on the following functions with the vertical mirror operator: $\hat{\sigma}_v f(x,y,z) = f(-x,-y,z)$? Is the function an eigenfunction of the operator? If so, what is the eigenvalue?

   (a) $f = \frac{x^2+y^2+z^4}{x+y+z}$

   (b) $f = xyz^2$

   (c) $f = xzy - z$

3. What is the result of operating on the following functions with the rotation operator: $\hat{C}_4 f(x,y,z) = f(y,-x,z)$? Is the function an eigenfunction of the operator? If so, what is the eigenvalue?

   (a) $f = \frac{x^2+y^2+z^4}{x+y+z}$

   (b) $f = xyz^2$

   (c) $f = xzy - z$

Exercises

4. Determine the point group of the following molecules

   (a) hydrogen peroxide

   (b) BrF_5

   (c) $Mn_2(CO)_{10}$ (Ask Drew Rutherford what this looks like)

   (d) trans-$PtCl_2Br_2$

(e) trans-$PtCl_2BrI$

(f) $Ni(CO)_4$

5. Treat the troublesome electron-electron interaction term in the Hamiltonian of helium as a perturbation to the Hamiltonian of helium without the electron electron interaction term whose wavefunctions are a product state of two hydrogen wavefunctions. Find the first order correction to energy.

6. Use perturbation theory to find the first order approximation to the ground state energy for a sextet oscillator ($V(x) = \frac{1}{2}kx^2 + \lambda x^6$). (Try to do this first by not looking at last year's problem set)

7. Use variational theory to estimate the ground state energy for a special quartic oscillator having potential
$$V(x) = x^4.$$
Use
$$\psi(x) = e^{-px^2}$$
as your trial wavefunction. Your algebraic equation for p will have several roots you will need to choose the correct one. Also make a plot of the optimized ground state wavefunction and $V(x)$. (For convenience set $\frac{\hbar^2}{2m}$ to one.) (Try to do this first by not looking at last year's problem set)

8. Construct the multiplication table of the D_{2h} point group. Verify the representations of x, y and z. Verify its direct product table.

9. Ethene is a D_{2h} molecule, sketch its normal modes and assign each mode to a representation.

Conceptual Problems

10. Consider each of the following systems. If you were to attack the problem using perturbation theory what model would you chose as the solvable system. Also state what the perturbative part of the Hamiltonian would account for.

    (a) The π electrons of a carbon nanotube in an external magnetic field

    (b) The quantum pendulum

    (c) A square quantum dot with a argon atom at its center

    (d) The quantum weeble

    (e) Hindered rotation

    (f) Particle in an rhombus

Reflective Exercises

11. Your graduate or medical training will likely cost the US tax payers as much as $250,000. I pay taxes, why should my tax dollars go towards your MS or Ph.D. degree?

12. Read the following condensed version of an essay entitled "Galileo and perspective: The art of renaissance science" by J.W. Dauben (APSNEWS Jan. 2002).

    (a) Do you think the cultural environment of a scientist influences the way that scientist approaches his or her work as a scientist?

    (b) Can you think of an example where the skills and techniques developed in art have been valuable in attacking a scientific problem?

Among the great figures of the Western scientific revolution of the 16th and 17th centuries—Copernicus, Kepler, Galileo, Descartes, Newton, Leibniz—all had at least one thing in common: they were all mathematicians. And yet, two stand out as being conspicuously different, for only Galileo and Newton were experimentalists. It was Galileo, at the beginning of the Scientific Revolution early in the 17th century, who demonstrated the extraordinary effectiveness of experimental observation of nature, coupled with analytical power of mathematics.

What Galileo achieved in revolutionizing physics was to show how observation, careful measurement, and attention to the structure of a given event all led to an appreciation of hidden causes that ultimately expressed the pervasive mathematical unity of all nature. Yet he was not the first to have done this, although in terms of astronomy and physics he was clearly a pioneer. Renaissance artists—painters, sculptors and architects—had been observing nature with a special interest in depicting it realistically from the early 15th century on. In fact, by turning to the problem of art and science in the Renaissance, it is possible to find what I believe are important roots for Galileo's own peculiarly realistic—and idealistic—approach to nature. For the values and attitudes Galileo held were ones he shared with Italian humanists, including philosophers, artisans, even musicians.

It is no coincidence, I think, that the artistic Renaissance and the scientific Renaissance should have both developed at first largely in Italy. Scientists like Galileo were doing exactly what Renaissance artists had been doing all along, with growing skill and increasingly sophisticated techniques, in their depictions of nature in realistic terms since the late 15th century. The veracity of their mathematical vision was well-established by the time Galileo began thinking about the mathematics—the geometry—of space nearly a century later. What Renaissance artists had discovered was that in addition to careful observation and attention to underlying physical structure—often this meant anatomical structure—mathematics was an especially useful tool for translating the physical reality of 3-dimensional objects in 3-dimensional space into realistic illusions of that same reality on only 2-dimensional, flat surfaces.

Galileo, like Renaissance artists of the 15th century, was interested in form, in the underlying reality of the natural world. He, too, was interested in the sort of physical reality that he felt his mathematics and the telescope were making clear for the first time. Light, optics, mathematics—all were as important keys for Galileo as they had been for Brunelleschi, Alberti and Piero della Francesca. From Plato Galileo took his faith in the ultimate rationality of nature, and the fact that the key to understanding nature was to be found in the ideal, perfect world of mathematics; but from Aristotle Galileo also understood that to understand nature, one must also be a systematic observer, and that it is only through experience and careful study of nature that the hidden secrets—the mathematical structures underlying the appearance of physical events and phenomena—can be discovered.

Galileo achieved a synthesis of observation and theory in a way that was strikingly modern and yet was also a product of the centuries of Italian humanism and the tremendous burst of energy we associate with the artistic Renaissance. New discoveries advanced the arts as well as the sciences, and many of these were due to new instruments and methods, especially ones related to mathematics.

1. (a) $\hat{i} f = \frac{x^2+y^2+z^4}{-x-y-z} = -1 f$ ungerade
   (b) $\hat{i} f = xyz^2 = 1f$ gerade
   (c) $\hat{i} f = -xyz + z = -1f$ ungerade

2. (a) $\sigma_v f = \frac{x^2+y^2+z^2}{-x-y+z}$ not eigenfunction
   (b) $\sigma_v f = xyz^2 = 1f$
   (c) $\sigma_v f = xyz - z = 1f$

3. (a) $\hat{C}_4 f = \frac{y^2+x^2+z^4}{y-x+z}$ not eigenfunction
   (b) $\hat{C}_4 f = -yxz^2 = -1f$
   (c) $\hat{C}_4 f = -xyz - z$ not eigenfunct.

4. (a) C_{2h} (b) C_{4v} (c) (d) D_{2h} (e) C_{6v} (f) T

5. $$\iiiiiint_{\text{all space}} \psi_{1s}^*(r_1)\psi_{1s}^*(r_2) \frac{e}{4\pi\epsilon|r_1 - r_2|} \psi_{1s}(r_1)\psi_{1s}(r_2)\, r_1^2 r_2^2 \sin\theta_1 \sin\theta_2 \, dr_1 dr_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

6. $\psi_0 = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2}\sqrt{\frac{km}{\hbar^2}} x^2}$

   $E_0^{(1)} = \int \psi_0^* \lambda x^6 \psi_0 \, dx = \frac{\lambda}{\pi}\int_{-\infty}^{\infty} x^6 e^{-\sqrt{\frac{km}{\hbar^2}} x^2} dx \xrightarrow{\text{mathematica}} \frac{15\lambda}{8\left(\frac{km}{\hbar}\right)^{7/4}\sqrt{\pi}}$

   $E_0 \simeq E_0^{(0)} + E_0^{(1)} = \hbar\omega\left(n + \frac{1}{2}\right) + \frac{15}{8\left(\frac{km}{\hbar}\right)^{7/4}\sqrt{\pi}}$

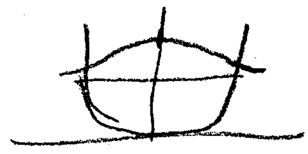
7. $E_{trial} = \frac{\int_{-\infty}^{\infty} \psi_{trial}^* H \psi_{trial}\, dx}{\int_{-\infty}^{\infty} \psi_{trial}^* \psi_{trial}} = \frac{\int_{-\infty}^{\infty} e^{-px^2}\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + x^4\right) e^{-px^2}}{\int_{-\infty}^{\infty} e^{-2px^2} dx}$

   set $\frac{\hbar^2}{2m} = 1$

   $E_{trial} = \frac{\frac{(3m + 16p^3)\sqrt{\frac{\pi}{2}}}{16p^{5/2}}}{\sqrt{\frac{\pi}{2p}}} = \frac{3 + 16p^3}{16p^3}$

   $\frac{dE_{trial}}{dp} = \frac{-3 + 8p^3}{8p^3} = 0 \Rightarrow$ only real root $p = \frac{(3)^{1/3}}{2}$

   $\psi = e^{-\frac{3^{1/3}}{2}x^2}$

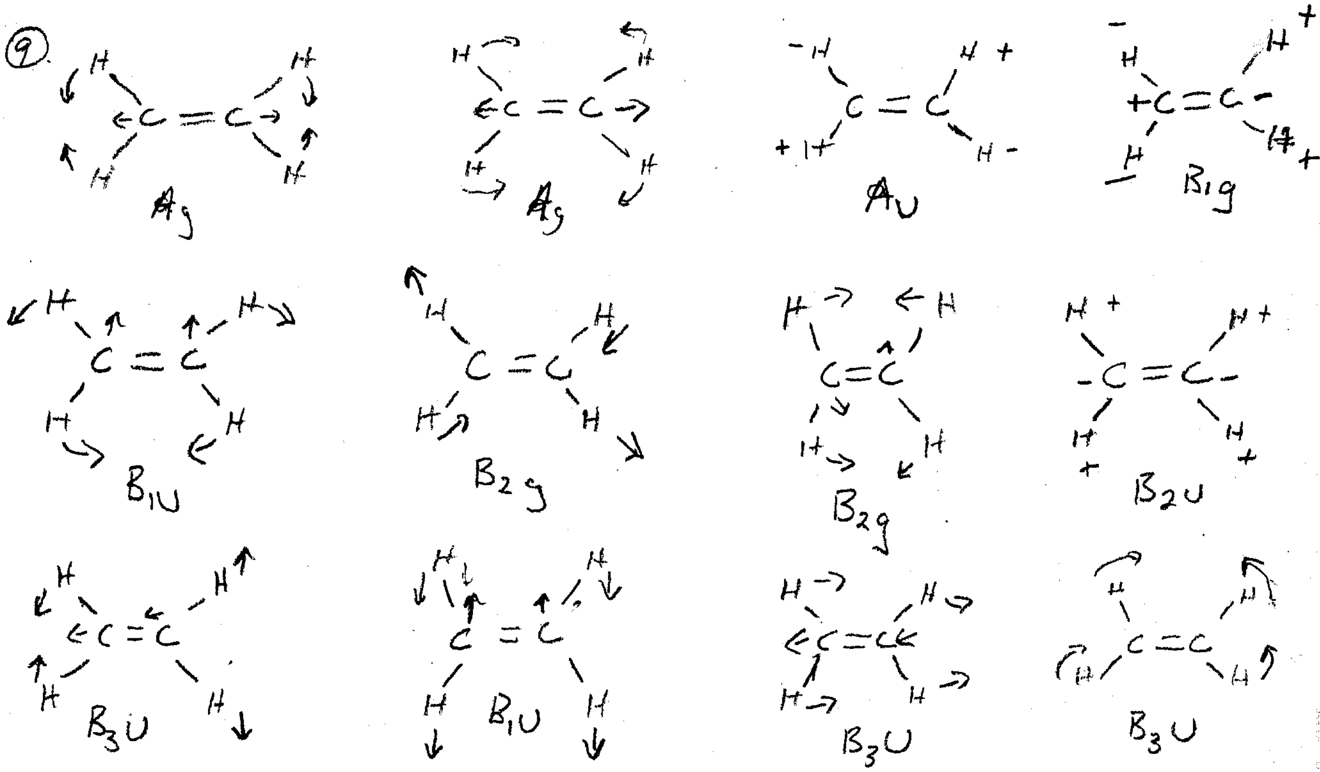


(8) your multiplication table

x, y, z do agree with the character table

direct product table agrees

(9)



(10)

	model	Perturbation
(a)	particle in a 1D box	magnetic field
(b)	HO	anharmonicity
(c)	particle in a 2D box	argon atom
(d)	HO	anharmonicity
(e)	HO	anharmonicity
(f)	particle in a 2D box	non-squareness