

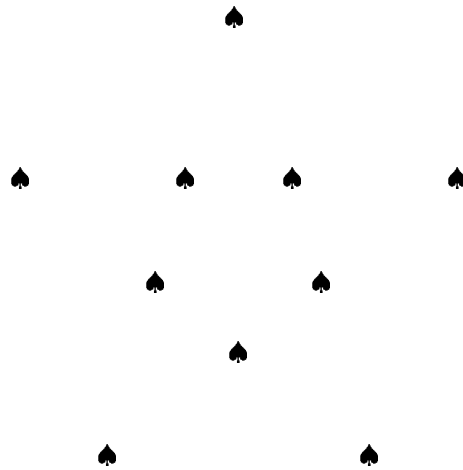
Quantum Mechanics Problems

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Introduction

Quantum Mechanics Problems (QMP) is a source book for instructors of introductory quantum mechanics. The book is available in electronic form to instructors by request to the author. It is free courseware and can be freely used and distributed, but not used for commercial purposes. The aim of QMP is to provide digestable problems for quizzes, assignments, and tests for modern students. There is a bit of spoon-finding—nourishing spoon-feeding I hope.

The problems are grouped by topics in chapters: see Contents below. The chapter ordering follows roughly the traditional chapter/topic ordering in quantum mechanics books. For each chapter there are two classes of problems: in order of appearance in a chapter they are: (1) multiple-choice problems and (2) full-answer problems. Almost all the problems have complete suggested answers. The answers may be the greatest benefit of QMP. The questions and answers can be posted on the web in pdf format.

The problems have been suggested by many sources, but have all been written by me. Given that the ideas for problems are the common coin of the realm, I prefer to call my versions of the problems redactions. Instructors, however, might well wish to find solutions to particular problems from well known texts. Therefore, I give the suggesting source (when there is one or when I recall what it was) by a reference code on the extra keyword line: e.g., (Gr-10:1.1) stands for Griffiths, p. 10, problem 1.1. Caveat: my redaction and the suggesting source problem will not in general correspond perfectly or even closely in some cases. The references for the source texts and other references follow the contents. A general citation is usually, e.g., Ar-400 for Arfken, p. 400.

At the end of the book are three appendices. The first is set of review problems anent matrices and determinants. The second is an equation sheet suitable to give to students as a test aid and a review sheet. The third is a set of answer tables for multiple choice questions.

Quantum Mechanics Problems is a book in progress. There are gaps in the coverage and the ordering of the problems by chapters is not yet final. User instructors can, of course, add and modify as they list.

Everything is written in plain T_EX in my own idiosyncratic style. The questions are all have codes and keywords for easy selection electronically or by hand. A fortran program for selecting the problems and outputting them in quiz, assignment, and test formats is also available. Note the quiz, etc. creation procedure is a bit clonky, but it works. User instructors could easily construct their own programs for problem selection.

I would like to thank the Department of Physics & Health Physics of Idaho State University for its support for this work. Thanks also to the students who helped flight-test the problems.

Contents

- 1 Classical Physics in Trouble
- 2 QM Postulates, Schrödinger Equation, and the Wave Function
- 3 Infinite Square Wells and Other Simple Wells
- 4 The Simple Harmonic Oscillator (SHO)
- 5 Free Particles and Momentum Representation
- 6 Foray into Advanced Classical Mechanics
- 7 Linear Algebra
- 8 Operators, Hermitian Operators, Bracket Formalism
- 9 Time Evolution
- 10 Measurement
- 11 The Central Force Problem and Orbital Angular Momentum

- 12 The Hydrogenic Atom
- 13 General Theory of Angular Momentum
- 14 Spin
- 15 Time-Independent Approximation Methods
- 16 Time-Dependent Perturbation
- 17 The Hydrogenic Atom and Spin
- 18 Multi-Particle Systems
- 19 Solids
- 20 Ephemeral Problems

Appendices

- 1 Mathematical Problems
- 2 Quantum Mechanics Equation Sheet
- 3 Multiple-Choice Problem Answer Tables

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Chapt. 1 Classical Physics in Trouble

Multiple-Choice Problems

001 qmult 00100 1 1 3 easy memory: quantum mechanics

1. The physical theory that deals mainly with microscopic phenomena is:
 - a) quartz mechanics.
 - b) quarks mechanics.
 - c) quantum mechanics.
 - d) quantum jump mechanics.
 - e) quasi-mechanics.

001 qmult 00200 1 1 1 easy memory: photon energy

2. The photon, the quantum of electromagnetic radiation, has **ENERGY**:
 - a) $hf = \hbar\omega$.
 - b) h/λ .
 - c) $\hbar k$.
 - d) $h^2 f$.
 - e) hf^2 .

001 qmult 00300 1 1 4 easy memory: photoelectric effect

3. A key piece of evidence for the wave-particle duality of light is:
 - a) the photograph effect.
 - b) the Maxwell's electrodynamics as summarized in the four Maxwell's equations.
 - c) the frequency of red light.
 - d) the photoelectric effect.
 - e) the photomagnetic effect.

001 qmult 00400 1 1 1 easy memory: Compton effect

4. Einstein predicted and Compton proved that photons:
 - a) have linear momentum.
 - b) do not have linear momentum.
 - c) sometimes have linear momentum.
 - d) both have and do not have linear momentum at the same time.
 - e) neither have nor have not linear momentum.

001 qmult 00500 1 4 3 easy deducto-memory: Bohr atom

5. "Let's play *Jeopardy!* For \$100, the answer is: This model of an atom is of historical and pedagogical interest, but it is of no use in modern practical calculations and from the modern standpoint is probably misleading rather than insight-giving."
 - a) What is Schrödinger's model of the hydrogen atom, Alex?
 - b) What the Thomas-Fermi model of a many electron atom, Alex?
 - c) What is Bohr's model of the hydrogen atom, Alex?

- d) What is the liquid drop model of the atom, Alex?
- e) What is model hydrogen atom of Leucippos and Democritus's , Alex?

001 qmult 00550 1 1 4 easy memory: hydrogenic energy formula

6. The formula

$$E_n = -\frac{1}{2}m_e c^2 \alpha^2 \frac{Z^2}{n^2}$$

gives the main energy levels of:

- a) positronium.
- b) magnesium deboride.
- c) the hydrogen molecule.
- d) the hydrogenic atom.
- e) the infinite square well.

001 qmult 00600 1 1 5 easy memory: Greek atomists

7. The atomic theory was first proposed by the ancient Greeks Leucippos (5th century BC) and Democritus (5th to 4th century BC: he reputedly lived to be 100). The term atomos means uncut: e.g., the grass is atomos. The atomists started from a philosophical position that there had to be something to give stability to nature: obviously the macroscopic world was full of change: therefore what was imperishable or uncuttable—atoms—must be below perception. The modern quantum theory does indeed bear out some of their thinking. Microscopic particles can be created and destroyed, of course, but the members of a class are much more identical than macroscopic objects can ever be: fundamental particles like electrons and quarks are thought to be absolutely identical. Thus the forms particles can take are apparently eternal: a hydrogen atom today is the same in theory as one at any time in universal history.

The atomists tried to work out an atomic understanding of existence in general. For instance they constructed a cosmology using atoms that bears some resemblance to modern eternal inflationary cosmology in which there are infinitely many universes that are born out of primordial space-time foam and perhaps return to that—foam to foam. Unfortunately, the atomists got off on the wrong foot on the shape of the Earth: they were still flat Earthers when the round Earth theory was being established. Quite obviously to us, the atomists were badly non-experimental. Much of their thinking can be called rational myth. To a degree they were lucky in happening to be attracted to an essentially right idea.

The atomists were eventually stigmatized as atheists: they did not deny that gods exist, but didn't leave anything for the gods to do. This may have been their downfall. The more orthodox and popular philosophies of Plato, Aristotle, and the Stoics rejected atomism probably, among other things, for its seeming atheism. Christianity followed suit in this regard. The writings of the atomists only exist in fragments—and Democritus seems to have been as famous as Plato in his day. The Epicurean philosophers adopted atomism, but also suffered the stigmatization as atheists—and also hedonists who are, of course, the worst. But the atom idea lingered on through the centuries: Leucippos and Democritus, Epicurus, Lucretius (his surviving poem *De Rerum Natura* [*On Nature*] expounds atomism), Gassendi (17th century), Newton, Dalton: the chain is unbroken: it is not true that modern atomism has no historical or essential connection to ancient atomism.

A good account of ancient atomism can be found in David Furley's *The Greek Cosmologists*.

Now, without recurring to the top of this preamble, atomism was invented in:

- a) the early 19th century.
- b) the 17th century by Gassendi.
- c) the 10th century AD.
- d) the 5th century AD.

- e) the 5th century BC.

001 qmult 00800 1 1 1 easy memory: causality, relativity

8. Einstein ruled out faster than light signaling because:
- a) it would cause irresolvable causality paradoxes.
 - b) it would not cause irresolvable causality paradoxes.
 - c) it led to irresolvable paradoxes in quantum mechanics.
 - d) it would destroy the universe.
 - e) it had been experimentally verified.

001 qmult 00900 1 1 3 easy memory: EPR paradox

9. The Einstein-Podolsky-Rosen (EPR) paradox was proposed to show that ordinary quantum mechanics implied superluminal signaling and therefore was:
- a) more or less correct.
 - b) absolutely correct.
 - c) defective.
 - d) wrong in all its predictions.
 - e) never wrong in its predictions.

001 qmult 01000 1 4 3 easy deducto-memory: Bell's theorem

10. "Let's play *Jeopardy!* For \$100, the answer is: This theorem (if it is indeed inescapably correct) and the subsequent experiments on the effect the theorem dealt with show that quantum mechanical signaling exceeds the speed of light."
- a) What is Dark's theorem, Alex?
 - b) What is Midnight's theorem, Alex?
 - c) What is Bell's theorem, Alex?
 - d) What is Book's theorem, Alex?
 - e) What is Candle's theorem, Alex?

Full-Answer Problems

001 qfull 00500 3 5 0 tough thinking: Rutherford's nucleus

Extra keywords: (HRW-977:62P)

1. Rutherford discovered the nucleus in 1911 by bombarding metal foils with alpha particles now known to be helium nuclei (atomic mass 4.0026). An alpha particle has positive charge $2e$. He expected the alpha particles to pass right through the foils with only small deviations. Most did, but some scattered off at very large angles. Using a classical particle picture of the alpha particles and the entities they were scattering off of he came to the conclusion that atoms contained most of their mass and positive charge inside a region with a size scale of $\sim 10^{-15}\text{m} = 1\text{ fm}$: this 10^{-5} times smaller than the atomic size. (Note fm stands officially for femtometer, but physicists call this unit a fermi.) Rutherford concluded that there must be a dense little core to an atom: the nucleus.
 - a) Why did the alpha particles scatter off the nucleus, but not off the electrons? **HINTS:** Think dense core and diffuse cloud. What is the force causing the scattering?
 - b) If the alpha particles have kinetic energy 7.5 MeV, what is their de Broglie wavelength?
 - c) The closest approach of the alpha particles to the nucleus was of order 30 fm. Would the wave nature of the alpha particles have had any effect? Note the wave-particle duality was not even suspected for the massive particles in 1911.

001 qfull 01000 3 5 0 tough thinking: black-body radiation, Wien law

Extra keywords: (Le-62) gives a sketch of the derivations

2. Black-body radiation posed a considerable challenge to classical physics which it was partially able to meet. Let's see how far we can get from a classical, or at least semi-classical, thermodynamic equilibrium analysis.

- a) Let U_λ be the radiation energy density per wavelength of a thermodynamic equilibrium radiation field trapped in some kind of cavity. The adjective thermodynamic equilibrium implies that the field is homogenous and isotropic. I think Hohlraum was the traditional name for such a cavity. Let's call the field a photon gas and be done with it—anachronism be darned. Since the radiation field is isotropic, the specific intensity is then given by

$$B(\lambda, T) = \frac{cU_\lambda}{4\pi} , \quad (\text{Pr.1})$$

where c is of course the speed of light. Specific intensity is radiation flux per wavelength per solid angle. From special relativity (although there may be some legitimately classical way of getting it), the momentum flux associated with a specific intensity is just $B(\lambda, T)/c$. Recall the rest plus kinetic energy of a particle is given by

$$E = \sqrt{p^2c^2 + m_0^2c^4} , \quad (\text{Pr.2})$$

where p is momentum and m_0 is rest mass. From an integral find the expression for the radiation pressure on a specularly reflecting surface:

$$p = \frac{1}{3}U , \quad (\text{Pr.3})$$

where p is now pressure and U is the wavelength-integrated radiation density. Argue that the same pressure applies even if the surface is only partially reflecting or pure blackbody provided the the radiation field and the surface are in thermodynamic equilibrium. **HINT:** Remember to account for angle of incidence and reflection.

- b) Now we can utilize a few classical thermodynamic results to show that

$$U = aT^4 , \quad (\text{Pr.4})$$

where a is a radiation constant related to the Stefan-Boltzmann constant $\sigma = 5.67051 \times 10^5 \text{ ergs}/(\text{cm}^2 \text{ K}^4)$ and T is Kelvin temperature, of course. The relation between a and σ follows from the find the flux leaking out a small hole in the Hohlraum:

$$F = 2\pi \int_0^1 \frac{cU}{4\pi} \mu d\mu = \frac{ca}{4} T^4 , \quad (\text{Pr.5})$$

where μ is the cosine of the angle to the normal of the surface where the hole is. One sees that $\sigma = ca/4$. Classically a cannot be calculated theoretically; in quantum mechanical statistical mechanics a can be derived. The proportionality $U \propto T^4$ can, however, be derived classically. Recall the 1st law of thermodynamics:

$$dE = T dS - p dV , \quad (\text{Pr.6})$$

where E is internal energy, S is entropy, and V is volume. Note that

$$\left(\frac{\partial E}{\partial S} \right)_V = T \quad \text{and} \quad \left(\frac{\partial E}{\partial V} \right)_S = -p , \quad (\text{Pr.7})$$

where the subscripts indicate the variables held constant. It follows from calculus (assuming well-behaved functions) that

$$\left(\frac{\partial p}{\partial S}\right)_V = -\left(\frac{\partial T}{\partial V}\right)_S, \quad (\text{Pr.8})$$

The last relation is one of Maxwell's four thermodynamic relations—Newton did things in threes; Maxwell in fours. Note that $E = UV$ for a radiation field. Now go to it: show $U \propto T^4$.

- c) As a by-product of the part (b) answer, you should have found that

$$T \propto V^{-1/3} \quad (\text{Pr.9})$$

for a quasistatic adiabatic process with the photon gas. (Find it now if somehow you missed it in the part (b) answer.) Assume you have a perfectly reflecting Hohlraum that you expand homologously by a scaling factor $f(t)$, where t is time. Thus at any time t any length ℓ between physical points on the walls in the system is given by

$$\ell = f(t)\ell_0, \quad (\text{Pr.10})$$

where ℓ_0 was the physical length at t_0 when $f(t_0) = 1$. Find out how T , U , $U dV$, and E scale with $f(t)$. What happens to the lost internal energy? **HINT:** This is easy.

- d) Consider the process described in the part (c) and show that

$$\lambda = \lambda_0 f(t) \quad (\text{Pr.11})$$

for each specific intensity beam. Note you can use the non-relativistic Doppler effect since the velocity shift between scatterings off the walls is vanishingly small in the quasistatic limit.

- e) For the same system as in part (c) show that

$$B(\lambda, T) d\lambda dV = f(t)^{-1} B(\lambda_0, T_0) d\lambda_0 dV_0. \quad (\text{Pr.12})$$

Then show that equation (Pr.12) leads naturally (if not absolutely necessarily so far as I can see) to the prescription for black-body specific intensity

$$B(\lambda, T) = \lambda^{-5} g(x) = \left(\frac{T}{x}\right)^5 g(x), \quad (\text{Pr.13})$$

where

$$x \equiv \lambda T \quad (\text{Pr.14})$$

and $g(x)$ is a universal function that cannot be determined from classical theory. Equation (Pr.13) is sometimes called Wien's displacement law. However the name Wien's displacement law is more usually (I think) reserved for the immediate result that for fixed T the the maximum of the black-body specific intensity (i.e., the maximum of $x^{-5}g(x)$) occurs at a wavelength given by

$$\lambda = \frac{x_{\max}}{T}, \quad (\text{Pr.15})$$

where x_{\max} is the global universal location of maximum for the universal function $g(x)$. It was empirically known that black-body radiation had only one maximum with wavelength, and so this corresponds to x_{\max} . I think classically x_{\max} has to be determined empirically.

Wien's radiation law was I believe a fit to the observations of Wien's displacement law. This law is

$$B(\lambda, T) = k_1 \left(\frac{T}{x}\right)^5 \exp\left(-\frac{k_2}{x}\right), \quad (\text{Pr.16})$$

where k_1 and k_2 had to be determined from the fit. Wien's law works well for short wavelengths ($x \lesssim x_{\max}$), but gives a poorish fit to the long wavelengths ($x \gtrsim x_{\max}$) (Pa-190, but note the x there is the inverse of the x here aside from a constant). The Rayleigh-Jeans law derived from a rather different classical starting picture gave a good fit to long wavelengths ($x \gg x_{\max}$), but failed badly at shorter wavelengths (Pa-190, but note the x there is the inverse of the x here aside from a constant). In fact the Rayleigh-Jeans law goes to infinity as x goes to zero and the total energy in a Rayleigh-Jeans radiation field is infinite (Le-64): this is sometimes called the ultraviolet catastrophe (BFG-106). The correct black-body specific intensity law was derived from a primitive quantum theory by Max Planck in 1900 (BFG-106). Planck obtained an empirically excellent fit to the black-body specific intensity and then was able to derive it from his quantum hypothesis. The Rayleigh-Jeans and Planck laws are the subject for another question.

001 qfull 01100 2 5 0 moderate thinking: Bohr atom

3. In 1913, Niels Bohr presented his model of the hydrogen atom which was quickly generalized to the hydrogenic atom (i.e., the one-electron atom of any nuclear charge Z). This model correctly gives the main hydrogenic atom energy levels and consists of a mixture of quantum mechanical and classical ideas. It is historically important for showing that quantization is somehow important in atomic structure and pedagogically it is of interest since it shows how simple theorizing can be done. But the model is, in fact, incorrect and from the modern perspective probably even misleading about the quantum mechanical nature of the atom. It is partially an accident of nature that it exists to be found. Only partially an accident since it does contain correct ingredients. And it is no accident that Bohr found it.

Bohr knew what he wanted: a model that would successfully predict the hydrogen atom spectrum which is a line spectrum showing emission at fixed frequencies. He knew from Einstein's photoelectric effect theory that electromagnetic radiation energy was quantized in amounts $h\nu$ where $h = 6.626 \times 10^{-27}$ erg s was Planck's constant (which was introduced along with the quantization notion to explain black-body radiation in 1900) and ν was frequency of the quantum of radiation. He recognized that Planck's constant had units of angular momentum. He knew from Rutherford's nuclear model of the atom that the positive charge of an atom was concentrated in region that was much smaller than the atom size and that almost all the mass of the atom was in the nucleus. He knew that there were negative electrons in atoms and they were much less massive than the nucleus. He knew the structure of atoms was stable somehow. By a judicious mixture of classical electromagnetism, classical dynamics, and quantum ideas he found his model. A more sophisticated mixture of these concepts would lead to modern quantum mechanics.

Let's see if we can follow the steps of the ideal Bohr—not the Bohr of history. **NOTE:** This is a semi-classical question: Bohr, ideal or otherwise, knew nothing of the Schrödinger equation in 1913.

- a) Bohr thought to build the electron system about the nucleus based on the electrostatic inverse square law with the electron system supported against collapse onto the nucleus by kinetic energy. The nucleus was known to be much more massive than the electron, and so could be considered an immobile center of force. The electron—there is only one in a hydrogenic atom—was taken to be in orbit about the nucleus. Circular orbits seemed the simplest way to proceed. The electrostatic force law (in Gaussian cgs units) in scalar form for a circular orbit is

$$F = -\frac{Ze^2}{r^2},$$

where Ze is the nuclear charge, e is the electron charge, and r is the radial distance between nucleus and electron. What is the potential energy of the electron with the zero of potential energy for the electron at infinity as usual? **HINT:** If the result isn't obvious, you can get

it using the work-potential energy formula:

$$V = - \int \vec{F} \cdot d\vec{r} + \text{constant} .$$

- b) Using the centripetal force law (which is really $f = ma$ for uniform circular motion)

$$F = - \frac{mv^2}{r} ,$$

find an expression for the classical kinetic energy T of the electron in terms of Z , e , and r alone.

- c) What is the total energy of the electron in the orbit?
- d) Classically an accelerating charge radiates. This seemed well established experimentally in Bohr's time. But an orbiting electron is accelerating, and so should lose energy continuously until it collapses into the nucleus: this catastrophe obviously doesn't happen. Electrons do not collapse into the nucleus. Also they radiate only at fixed frequencies which means fixed quantum energies by Einstein's photoelectric effect theory. So Bohr postulated that the electron could only be in certain orbits which he called stationary states and that the electron in a stationary state did not radiate. Only on transitions between stationary states was there an emission of radiation in a quantum or (to use an anachronism) a photon. To get the fixed energies of emission only certain energies were allowed for the stationary states. But the emitted photons didn't come out with equally spaced energies: ergo the orbits couldn't be equally spaced in energy. From the fact that Planck's constant h has units of angular momentum, Bohr hypothesized the orbits were quantized in equally spaced amounts of angular momentum. But h was not the spacing that worked. Probably after a bit of fooling around, Bohr found that $h/(2\pi)$ or, as we now write it, \hbar was the spacing that gave the right answer. The allowed angular momenta were given by

$$L = n\hbar ,$$

where n is any positive non-zero integer. The n was the first quantum number: we now call it the principal quantum number. It indeed determines the main spacing of the hydrogenic energy levels. Rewrite kinetic energy T in terms of $n\hbar$ and solve for an expression for r in terms n , \hbar , Ze^2 and m only. **HINT:** Recall the classical expression for angular momentum of particle in a circular orbit is $L = mrv$.

- e) Using the formula for r from the part (d) answer write an expression for the energy of a stationary state in terms of m , c , α , Z , and n only. The c is the speed of light and the α is the fine structure constant: in Gaussian cgs units

$$\alpha = \frac{e^2}{\hbar c} .$$

(Real physicists use Gaussian cgs units). This formula for orbit energy turns out to be correct for the spacing of the main energy levels or shells as we would now call them. But a shell doesn't, in fact, have angular momentum $n\hbar$: it consists of has orbitals (as we now call them) with angular momenta in the range $[0, n-1]$ in units of \hbar (e.g., Gr-139).

001 qfull 01300 2 3 0 moderate math: Compton scattering

Extra keywords: (Ha-323:1.1)

4. In 1916, Einstein proposed that photons carry momentum according to the following formula:

$$p = \frac{h}{\lambda} ,$$

where h is Planck's constant and λ is the photon wavelength (HRW-959). In 1924, Louis de Broglie applied the formula in inverse form to give a wavelength for massive particles: i.e.,

$$\lambda = \frac{h}{p}$$

which is called the de Broglie wavelength formula. In 1923, Arthur Compton carried out experiments with X-rays scattering off electrons which showed that Einstein's formula correctly accounted for the wavelength shift on scattering. The Compton shift formula is

$$\Delta\lambda = \lambda_C(1 - \cos\theta) ,$$

where $\lambda_C = h/(m_e c) = 0.02426 \text{ \AA}$ is the Compton wavelength (with m_e being the electron mass) and θ is the scattering angle (i.e., the angle between incident and scattering directions). This formula can be derived from Einstein's formula using a relativistic particle collisional picture.

- a) Assuming an electron starts at rest and is hit head-on by a photon “particle and the collision is elastic,” what conservation law expressions can be used to relate incoming photon momentum p_1 , outgoing photon momentum p_2 , outgoing electron momentum p_e , photon scattering angle θ , and electron scattering angle ϕ ? Can one solve for the four outgoing quantities given the initial conditions? **HINT:** Recall that the relativistic kinetic energy of a particle is given by

$$T = \sqrt{(pc)^2 + (m_0 c^2)^2} - m_0 c^2 = (\gamma - 1)m_0 c^2 ,$$

where p is momentum and m_0 is the rest mass.

- b) Solve for p_2 in terms of p_1 and θ only.
 c) Now using Einstein wavelength formula, find Compton's formula.
 d) Sketch the behavior of $\Delta\lambda$ as a function of θ . What is the shift formula in the non-relativistic limit: i.e., when $\lambda \rightarrow \infty$.

001 qfull 00150 3 5 0 tough thinking: Einstein, Runyon

5. “God does not play dice”—Einstein. Discuss.

Chapt. 2 QM Postulates, Schrödinger Equation, and the Wave Function

Multiple-Choice Problems

002 qmult 00080 1 1 2 easy memory: wave-particle duality

1. The principle that all microscopic physical entities have both wave and particle properties is called:
 - a) the wave-particle singularity.
 - b) the wave-particle duality.
 - c) the wave-particle triality.
 - d) the wave-particle infinality.
 - e) the wave-particle nullity.

002 qmult 00090 1 4 5 easy deducto-memory: Schrödinger eqn

2. "Let's play *Jeopardy!* For \$100, the answer is: The equation that governs the time evolution of quantum mechanical systems in the non-relativistic approximation."
 - a) What is $\vec{F}_{\text{net}} = m\vec{a}$, Alex?
 - b) What are Maxwell's equations, Alex?
 - c) What are Einstein's field equations of general relativity, Alex?
 - d) What is the Dirac equation, Alex?
 - e) What is Schrödinger's equation, Alex?

002 qmult 00100 1 1 1 easy memory: Schrödinger's eqn. compact form

3. The full Schrödinger's equation in compact form is:
 - a) $H\Psi = i\hbar(\partial\Psi/\partial t)$.
 - b) $H\Psi = \hbar(\partial\Psi/\partial t)$.
 - c) $H\Psi = i(\partial\Psi/\partial t)$.
 - d) $H\Psi = i\hbar(\partial\Psi/\partial x)$.
 - a) $H^{-1}\Psi = i\hbar(\partial\Psi/\partial t)$.

002 qmult 00200 1 1 5 easy memory: probability of finding particle in dx

4. The probability of finding a particle in differential region dx is:
 - a) $\Psi(x, t) dx$.
 - b) $\Psi(x, t)^* dx$.
 - c) $[\Psi(x, t)^*/\Psi(x, t)] dx$.
 - d) $\Psi(x, t)^2 dx$.
 - e) $\Psi(x, t)^* \Psi(x, t) dx = |\Psi(x, t)|^2 dx$.

002 qmult 00210 1 1 1 easy memory: QM probability density

5. In the statistical interpretation of wave function Ψ , $|\Psi|^2$ is:
 - a) a probability density.
 - b) a probability amplitude.
 - c) 1.

- d) 0.
- e) a negative probability.

002 qmult 00300 1 1 3 easy memory: expectation value defined

6. The expectation value of a dynamical quantity is:
- a) the most likely value of the quantity given by the probability density: i.e., the mode of the probability density.
 - b) the median value of the quantity given by the probability density.
 - c) the mean value of the quantity given by the probability density.
 - d) any value you happen to measure.
 - e) the time average of the quantity.

002 qmult 00310 1 1 3 easy memory: expectation value expression

7. The expectation value of operator Q for some wave function is often written:
- a) Q
 - b) $\rangle Q \langle$.
 - c) $\langle Q \rangle$.
 - d) $\langle f(Q) \rangle$
 - e) $f(Q)$.

002 qmult 00400 1 1 4 easy memory: normalization requirement

8. A physical requirement on wave functions is that they should be:
- a) reliable
 - b) friable.
 - c) certifiable.
 - d) normalizable.
 - e) retrievable.

002 qmult 00500 1 1 2 easy memory: the momentum operator defined

9. The momentum operator in one-dimension is
- a) $\hbar \frac{\partial}{\partial x}$.
 - b) $\frac{\hbar}{i} \frac{\partial}{\partial x}$.
 - c) $\frac{i}{\hbar} \frac{\partial}{\partial x}$.
 - d) $\frac{i}{\hbar} \frac{\partial}{\partial t}$.
 - d) $\hbar \frac{\partial}{\partial t}$.

002 qmult 00510 1 1 4 easy memory: constant of the motion

10. If an operator has no explicit time dependence and it commutes with the Hamiltonian, then it is a quantum mechanical:
- a) fudge factor.
 - b) dynamical variable.
 - c) universal constant.
 - d) constant of the motion.
 - e) constant of the stagnation.

002 qmult 00520 1 4 5 easy deducto-memory: Ehrenfest's theorem

11. Ehrenfest's theorem partially shows the connection between quantum mechanics and:
- a) photonics

- b) electronics.
- c) special relativity.
- d) general relativity.
- e) classical mechanics.

002 qmult 00520 1 4 5 easy deducto-memory: Heisenberg uncertainty

12. “Let’s play *Jeopardy!* For \$100, the answer is: It describes a fundamental limitation on the accuracy with which we can know position and momentum simultaneously.”
- a) What is Tarkovsky’s doubtful thesis, Alex?
 - b) What is Rublev’s ambiguous postulate, Alex?
 - c) What is Kelvin’s vague zeroth law, Alex?
 - d) What is Schrödinger’s wild expostulate, Alex?
 - e) What is Heisenberg’s uncertainty principle, Alex?

002 qmult 00600 1 4 5 easy deducto-memory: uncertainty principle

13. “Let’s play *Jeopardy!* For \$100, the answer is: $\sigma_x \sigma_p \geq \hbar/2$.”
- a) What is an equality, Alex?
 - b) What is a standard deviation, Alex?
 - c) What is the Heisenberg **CERTAINTY** principle, Alex?
 - d) What is the Cosmological principle, Alex?
 - e) What is the Heisenberg **UNCERTAINTY** principle, Alex?

002 qmult 00700 1 1 4 easy memory: Schr. eqn. separation of variables

14. The time-independent Schrödinger equation is obtained from the full Schrödinger equation by:
- a) colloquialism.
 - b) solution for eigenfunctions.
 - c) separation of the x and y variables.
 - d) separation of the space and time variables.
 - e) expansion.

002 qmult 00720 1 1 1 easy memory: stationary state

15. A system in a stationary state will:
- a) not evolve in time.
 - b) evolve in time.
 - c) both evolve and not evolve in time.
 - d) occasionally evolve in time.
 - e) violate the Heisenberg uncertainty principle.

002 qmult 00800 1 4 2 easy deducto-memory: orthogonality property

16. For an eigenproblem, one can always find a complete set of eigenfunctions that are:
- a) independent of the x -coordinate.
 - b) orthonormal.
 - c) collinear.
 - d) pathological.
 - e) righteous.

002 qmult 00900 1 4 1 easy deducto-memory: macro object in stationary state

17. “Let’s play *Jeopardy!* For \$100, the answer is: A state that no macroscopic system can be in although some might argue that Bose-Einstein condensates and other special systems like superconductors and superfluids can be sort of.”

- a) What is a stationary state, Alex?
- b) What is an accelerating state, Alex?
- c) What is a state of the Union, Alex?
- d) What is a state of being, Alex?
- e) What is a state of mind, Alex?

002 qmult 01000 1 1 5 easy memory: stationary state is radical

18. A stationary state is:

- a) just a special kind of classical state.
- b) more or less a kind of classical state.
- c) voluntarily a classical state.
- d) was originally not a classical state, but grew into one.
- e) radically unlike a classical state.

002 qmult 01100 1 1 4 easy memory: macro system in a stationary state

19. Except for certain special cases (superconductors, superfluids, and Bose-Einstein condensates), no macroscopic system can be in a:

- a) mixed state.
- b) vastly mixed state.
- c) classical state.
- d) stationary state.
- e) state of the union.

002 qmult 01200 1 1 2 easy memory: transitions

20. Transitions between stationary states (sometimes, but actually rarely, called quantum jumps) are:

- a) only collisional.
- b) both collisional and radiative.
- c) only radiative.
- d) neither collisional nor radiative.
- e) only collisional to higher energy stationary states and only radiative to lower energy stationary states.

002 qmult 01300 1 4 3 easy deducto-memory: lasers, stimulated emission

21. "Let's play *Jeopardy!* For \$100, the answer is: It is the basis for lasers and masers."

- a) What spontaneous radiative emission, Alex?
- b) What desultory radiative emission, Alex?
- c) What stimulated radiative emission, Alex?
- d) What the laser force, Alex?
- e) What the laser potential, Alex?

002 qmult 01400 1 4 4 easy deducto-memory: operators and Sch. eqn.

22. "Let's play *Jeopardy!* For \$100, the answer is: An equation that must hold in order for the non-relativistic Hamiltonian operator and the operator $i\hbar\partial/\partial t$ to both represent energy in the evaluation of the energy expectation value for a wave function $\Psi(x, t)$."

- a) What is the continuity equation, Alex?
- b) What is the Laplace equation, Alex?
- c) What is Newton's law, Alex?
- d) What is Schrödinger's equation, Alex?
- e) What is Hamilton's equation, Alex?

002 qmult 02000 2 1 4 moderate memory: does gravity quantize

Extra keywords: reference: Nesvizhevsky et al. 2002, Nature, 413, 297

23. Can the gravitational potential cause quantization of energy states?

- a) No.
- b) It is completely uncertain.
- c) Theoretically yes, but experimentally no.
- d) Experimental evidence to date (post-2001) suggests it can.
- e) In principle there is no way of telling.

Full-Answer Problems

002 qfull 00090 1 5 0 easy thinking: what is a wave function?

1. What is a wave function? (Representative general symbol $\Psi(\vec{r}, t)$).

002 qfull 00100 1 3 0 easy math: probability and age distribution

Extra keywords: (Gr-10:1.1)

2. Given the following age distribution, compute its the normalization (i.e., the factor that normalizes the distribution), mean, variance, and standard deviation. Also give the mode (i.e., the age with highest frequency) and median.

Table: Age Distribution

Age (years)	Frequency
14	2
15	1
16	6
22	2
24	2
25	5

002 qfull 00200 2 3 0 moderate math: probability needle I

Extra keywords: (Gr-10:1.3) probability and continuous variables

3. An indicator needle on a semi-circular scale (e.g., like a needle on car speedometer) bounces around and comes to rest with equal probability at any angle θ in the interval $[0, \pi]$.
 - a) Give the probability density $\rho(\theta)$ and sketch a plot of it.
 - b) Compute the 1st and 2nd moments of the distribution (i.e., $\langle \theta \rangle$ and $\langle \theta^2 \rangle$) and the variance and standard deviation.
 - c) Compute $\langle \sin \theta \rangle$, $\langle \cos \theta \rangle$, $\langle \sin^2 \theta \rangle$, and $\langle \cos^2 \theta \rangle$.

002 qfull 00210 3 5 0 tough thinking: 2-variable probability density

Extra keywords: (Gr-11:1.5) dropping a needle on lines

4. Nun für eine kleine teufelische problem. Say you drop at random with equal likelihood of landing in any orientation and location a needle of length ℓ onto a sheet of paper with parallel lines a distance ℓ apart. What is the probability of the needle crossing (or at least touching) a line? Let's be nice this time and break it down.

- a) Mentally mark one end of needle red. Then note that really we only need to consider one band on the paper between two parallel lines and the case where the red end lies between them as a given. Why is this so?
- b) So now we consider that the red end lands in one band at a point x between $-\ell/2$ and $\ell/2$. Note we put the origin at the center since almost always one ought to exploit symmetry. What is the probability density for the red end to land anywhere in the band? What is the probability density for the needle for the orientation of the needle in θ measured from the x -axis? Why do you only need to consider $\theta \in [0, \pi]$?
- c) Now we don't care about the orientation itself really: we just care about its projection on the x -axis. Call that projection x' . What is the probability density for x' ? What is the range of x' allowed? **HINT:** The probability of landing in $d\theta$ and a corresponding dx' must be equal.
- d) The joint probability density for x and x' is

$$\rho(x)\rho(x') .$$

You now have to integrate up all the probability for $x' + x \geq \ell/2$ and for $x' + x \leq -\ell/2$ and sum those two probabilities. The sum is the solution probability of course.

002 qfull 00220 1 3 0 easy math: Gaussian probability density

Extra keywords: (Gr-11:1.6)

5. Consider the Gaussian probability density

$$\rho(x) = Ae^{-\lambda(x-a)^2} ,$$

where A , a , and λ are constants.

- a) Determine the normalization constant A .
- b) The n th moment of a probability density is defined by

$$\langle x^n \rangle = \int_{-\infty}^{\infty} x^n \rho(x) dx .$$

Determine the 0th, 1st, and 2nd moments of the Gaussian probability density.

- c) For the Gaussian probability density determine the mean, mode, mediam, variance σ^2 , and standard deviation (or dispersion) σ .
- d) Sketch the Gaussian probability density.

002 qfull 00300 2 3 0 moderate math: analyzing a triangular hat wave function

Extra keywords: (Gr-13:1.7)

6. At some time a triangular hat wave function is given by

$$\Psi(x, t) = \begin{cases} A\frac{x}{a} , & x \in [0, a]; \\ A\left(\frac{b-x}{b-a}\right) , & x \in [a, b]; \\ 0 & \text{otherwise,} \end{cases}$$

where A , a , and b are constants.

- a) Sketch Ψ and locate most probable location for a particle (i.e., the mode of the $|\Psi|^2$ probability distribution).

- b) Determine the normalization constant A in terms of a and b . Recall the difference between wave function and probability distribution here and in the later parts of this question.
- c) What are the probabilities of being found left and right of a , respectively?
- d) What is $\langle x \rangle$?

002 qfull 00310 2 5 0 moderate thinking: probability conservation

Extra keywords: (Gr-13:1.9) probability current

- 7. The expression for the probability that a particle is in the region $[-\infty, x]$ (i.e., what one can call the probability function) is

$$P(x, t) = \int_{-\infty}^x |\Psi(x', t)|^2 dx' .$$

- a) Find an explicit, non-integral expression for $\partial P(x, t)/\partial t$ given that the wave function is normalizable at time t . **HINT:** Make use of the physics: i.e., the Schrödinger equation itself. This is a common trick in quantum mechanics and, mutatis mutandis, throughout physics.
- b) If the wave function is normalizable at time t , show that $P(\infty, t)$ is a constant with respect to time: i.e., total probability is conserved.
- c) The probability current is defined

$$J(x, t) = -\frac{\partial P(x, t)}{\partial t} .$$

Argue that this is a sensible definition.

- d) Given

$$\Psi(x, t) = \psi(x)e^{-i\omega t} ,$$

what can one say about the probability density $|\Psi|^2$, the probability function $P(x, t)$, and the probability current $J(x, t)$?

002 qfull 00320 3 5 0 tough thinking: general time evolution equation

- 8. By postulate the expectation value of an operator Q is given by

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^* Q \Psi dx .$$

- a) Write down the explicit expression for

$$\frac{d\langle Q \rangle}{dt} .$$

Recall Q in general can depend on time too.

- b) Now use the Schrödinger equation

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

to eliminate partial time derivatives where possible in the expression for $d\langle Q \rangle/dt$. Remember how complex values behave when complex conjugated. You should use the angle bracket form for expectation values to simplify the expression where possible.

- c) The commutator of two operators A and B is defined by

$$[A, B] = AB - BA ,$$

where it is always understood that the commutator and operators are acting on an implicit general function to the right. If you have trouble initially remembering the understood condition, you can write

$$[A, B]f = (AB - BA)f ,$$

where f is an explicit general function. Operators don't in general commute: i.e., $[A, B] = AB - BA \neq 0$ in general. Prove

$$\left[\sum_i A_i, \sum_j B_j \right] = \sum_{i,j} [A_i, B_j] .$$

- d) Now show that $d\langle Q \rangle/dt$ can be written in terms of $\langle i[H, Q] \rangle$. The resulting important expression oddly enough doesn't seem to have a common name. I just call it the general time evolution formula. **HINTS:** First, V and Ψ^* do commute. Second, the other part of the Hamiltonian operator

$$T = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

can be put in the right place using integration by parts and the normalization condition on the wave function. Note T turns out to be the kinetic energy operator.

- e) If $d\langle Q \rangle/dt = 0$, then Q is a quantum mechanical constant of the motion. Show that the operator $Q = 1$ (i.e., the unit operator) is a constant of the motion. What is $\langle 1 \rangle$?
- f) Find the expression for $d\langle x \rangle/dt$ in terms of what we are led to postulate as the momentum operator

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} .$$

The position operator x should be eliminated from the expression. **HINTS:** Note V and x commute, but T and x do not. The biderivative formula might be of use in evaluating the commutator $[T, x]$:

$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^n \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}} .$$

002 qfull 00330 3 5 0 tough thinking: Ehrenfest's theorem

Extra keywords: (Gr-17:1.12) Ehrenfest formulae

9. In one dimension Ehrenfest's theorem is usually taken to consist of two formulae:

$$\frac{d\langle x \rangle}{dt} = \frac{1}{m} \langle p \rangle$$

and

$$\frac{d\langle p \rangle}{dt} = - \left\langle \frac{\partial V}{\partial x} \right\rangle .$$

- a) From the general time evolution formula prove the 1st Ehrenfest formula. Recall the momentum operator is postulated to be given by

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} .$$

The biderivative formula might be of use in evaluating the commutator $[T, x]$:

$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^n \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}}.$$

- b) From the general time evolution formula prove the 2nd Ehrenfest formula. **HINTS:** Note that $[T, p] = 0$: i.e., T and p commute.
- c) If you invoke the correspondence principle (which in this case means scrunch the non-zero region of wave function into a macroscopic point or a Dirac-Delta-like function), what do the Ehrenfest formulae become in the macroscopic limit where $\langle x \rangle$ becomes x , etc? What does this result imply?
- d) If one combines the two Ehrenfest formulae, one gets

$$m \frac{d^2 \langle x \rangle}{dt} = - \left\langle \frac{\partial V}{\partial x} \right\rangle$$

which looks very like Newton's 2nd law in its $F = ma$ form for a force given by a potential. By the correspondance principle it does become the 2nd law in the macroscopic limit. However, an interesting question arises—well maybe not all that interesting. Does the $\langle x \rangle$ (which we could call the center of the wave packet) actually obey Newton's 2nd law according to the expression

$$m \frac{d^2 \langle x \rangle}{dt} = - \frac{\partial V(\langle x \rangle)}{\partial \langle x \rangle}$$

in general To disprove a general statement, all you need to do is find one counterexample. Consider a potential of the form $V(x) = Ax^\lambda$, and show that in general the $\langle x \rangle$ doesn't obey Newton's 2nd law in the form given. Then show that it does in three special cases of λ .

002 qfull 00400 1 3 0 easy math: orthonormality leads to mean energy

Extra keywords: (Gr-30:2.10)

- 10. You are given a complete set of orthonormal stationary states (i.e., energy eigenfunctions) $\{\psi_n\}$ and a general wave equation $\Phi(x, t)$ for the same system: i.e., $\Phi(x, t)$ is determined by the same Hamiltonian as the complete set. Find the general expression, simplified as far as possible, for expectation value $\langle H^\ell \rangle$ where ℓ is any positive (or zero) integer. Give the special cases for $\ell = 0, 1$, and 2 , and the expression for σ_E . **HINTS:** Use expansion and orthonormality. This should be a very short answer: 3 or 4 lines.

002 qfull 00500 3 5 0 tough thinking: real eigen-energies

Extra keywords: (Gr-24:2.1) and all real complete sets

- 11. There are a few simple theorems one can prove about stationary states and their eigen-energies.
 - a) Prove that eigen-energies must be real. **HINT:** Prove $\langle H \rangle$ is real for any state Ψ using integration by parts. Note one has to use the full time dependent wave function for a general state since the time dependence doesn't cancel out of the expectation value integral.
 - b) The complete set of time-independent stationary states you get from a direct solution of the Schrödinger equation may not be all pure real pure. But one can always construct from this complete set another complete set that is all pure real and it is supposedly convenient to do so sometimes—or at least it can be done as a mathematician would say. Show how it can be done. **HINTS:** First note that complete sets are almost always assumed to be minimum complete sets: i.e., each member of the set is independent of all the other members, and thus cannot be constructed from any linear combination of the others. In our discussions we always assume minimum complete sets.

Consider a non-trivially complex solution ψ_{ij} of the eigenproblem

$$H\psi_{ij} = E_i\psi_{ij} ,$$

where the first subscript denotes energy level and the second the particular solution of that energy level. (“Non-trivially” just means that ψ_{ij} isn’t just a real function times a complex constant. What do you do with a trivially complex ψ_{ij} by the way?) Take the complex conjugate of the eigenproblem to find an independent 2nd solution ψ_{2nd} to it with the same energy. The 2nd solution may or may not be part of your original subset with energy E_i . If it is, then that is good. But if it isn’t one of the original subset with energy E_i , you should replace one of those with ψ_{2nd} . Since the original set was complete

$$\psi_{2nd} = \sum_{\ell} c_{\ell} \psi_{i\ell} ,$$

where the summation only needs to run over the eigenfunctions with the same energy E_i . This equation can be rearranged for any ψ_{im} (except for ψ_{ij} itself):

$$\psi_{im} = \sum_{\ell} c_{\ell \neq m} \psi_{i\ell} + c \psi_{2nd} ,$$

where the coefficients c_{ℓ} all had to be changed and c is the coefficient needed for ψ_{2nd} . Since ψ_{im} can be constructed using ψ_{2nd} , it can be replaced by ψ_{2nd} . If the number of states with energy E_i is infinite, the replacement process becomes hairy, but let’s not worry about that.

Now construct two pure real solutions from ψ_{ij} and ψ_{2nd} from which ψ_{ij} and ψ_{2nd} can be re-constructed. These two new states then replace ψ_{ij} and ψ_{2nd} in the subset with energy E_i . One can go on like that replacing two for two as long as you need to. Remember the original set will in general be infinite, and one couldn’t have had them all explicitly anyway.

002 qfull 00600 3 5 0 tough thinking: parity operator

12. The parity operator P (not to be confused with the momentum operator p) has the well defined, but seemingly arbitrary, property that

$$Pf(x) = f(-x)$$

for a 1-dimensional case which is all that we will consider in this problem.

- a) Prove the parity operator is Hermitian. **HINTS:** Recall that the definition of the Hermitian conjugate of operator Q is

$$\langle \phi | Q | \psi \rangle = \langle \psi | Q^{\dagger} | \phi \rangle^* ,$$

where $|\phi\rangle$ and $|\psi\rangle$ are arbitrary kets. Note Q is Hermitian if $Q^{\dagger} = Q$. Since the parity operator (as defined here) only has meaning in the position representation that is where the proof must be done: thus one must prove

$$\int_{-\infty}^{\infty} \phi(x)^* P\psi(x) dx = \left[\int_{-\infty}^{\infty} \psi(x)^* P\phi(x) dx \right]^* .$$

A transformation of the integration variable might help: remember x in the integrals is just a dummy variable that can be represented by any symbol.

- b) The eigenproblem for the parity operator is

$$Pf(x) = p_{\text{val}} f(x) ,$$

where p_{val} are the eigenvalues. Solve for the complete set of eigenvalues and identify those classes of functions which are eigenfunctions of P . **HINTS:** Note it's $f(x)$ on the right hand side not $f(-x)$ since this is an eigenproblem, but $Pf(x) = f(-x)$ too. Recall that the eigenvalues of a Hermitian operator are pure real. Nothing forbids using the parity operator twice. The parity operator commutes with constants of course:

$$P[cf(x)] = cf(-x) = cPf(x) .$$

- c) The set of all eigenfunctions of P is complete. Thus P qualifies as an “observable” in QM jargon whether it can be observed or not: i.e., it is a Hermitian operator with a complete set of eigenstates. Show that the set of eigenstates is complete: i.e., that any function $f(x)$ can be written in an expansion of P eigenfunctions. **HINTS:** From any $f(x)$ one can construct another function $f(-x)$ and from $f(x)$ and $f(-x)$ one can construct two eigenfunctions of P , and from those two eigenfunctions of P one can reconstruct ...
- d) If $f'(x)$ is the derivative of $f(x)$, then $Pf'(x) = f'(-x)$: i.e., the derivative of $f(x)$ evaluated at $-x$. But what is

$$\frac{\partial}{\partial x}[Pf(x)] ?$$

Do P and $\partial/\partial x$ commute? Do P and $\partial^2/\partial x^2$ commute? **HINT:** You've heard of the chain rule.

- e) If the potential is even (i.e., $V(x) = V(-x)$) do P and the Hamiltonian H commute? **HINTS:** Recall $PV(x)f(x)$ must be interpreted in QM (unless otherwise clarified) as P acting on the function $V(x)f(x)$ not on $V(x)$ alone.
- f) Given that P and H commute and $\psi(x)$ is a solution of the time-independent Schrödinger equation, show that $\psi(-x)$ a solution too with the same eigen-energy as $\psi(x)$: i.e., $\psi(x)$ and $\psi(-x)$ are degenerate eigenstates.
- g) Given that P and H commute, show how one can construct from a given complete set of energy eigenstates a complete set of energy eigenstates that are also eigenstates of the parity operator. Assume that the original complete set contains both $\psi(x)$ and $\psi(-x)$: this is not a requirement for finding a common complete set, but it is a simplification here. **HINT:** Recall the part (c) answer.

002 qfull 01000 2 5 0 moderate thinking: energy and normalization

Extra keywords: (Gr-24:2.2) zero-point energy

13. Classically $E \geq V_{\min}$ for a particle in a conservative system.

- a) Show that this classical result must be so. **HINT:** This shouldn't be a from-first-principles proof: it should be about one line.
- b) The quantum mechanical analog is almost the same: $\bar{E} = \langle H \rangle > V_{\min}$ for any state of the system considered. Note the equality $\bar{E} = \langle H \rangle = V_{\min}$ never holds quantum mechanically. (There is an exception we will not consider in detail here. The lowest energy stationary state of a system with periodic boundary conditions and a flat potential can have $E = V_{\min}$. I don't real full periodic boundary conditions can exist for a 3-dimensional system in 3-d Euclidean space. But 1-d and 2-d systems with full periodic boundary conditions can exist: e.g., a ring and a sphere.) Prove the inequality. **HINTS:** The key point is to show that $\langle T \rangle > 0$ for all physically allowed states (except for the periodic boundary conditions exception). Use integration by parts.
- c) Now show that result $\bar{E} > V_{\min}$ implies $E > V_{\min}$, where E is any eigen-energy of the system considered. Note the equality $E = V_{\min}$ never holds quantum mechanically (except

for the periodic boundary conditions exceptions). In an ordinary sense there is no rest state for quantum mechanical particle. This lowest energy is often called the zero-point energy.

- d) The $E > V_{\min}$ result for an eigen-energy in turn implies a 3rd result: any ideal measurement always yields an energy greater than V_{\min} (except for the periodic boundary condition exception). Prove this by reference to a quantum mechanical postulate.

002 qfull 00110 2 5 0 moderate thinking: beyond the classical turning points

14. The constant energy of a classical particle in a conservative system is given by

$$E = T + V .$$

Since classically $T \geq 0$ always, a bound particle is confined by surface defined by $T = 0$ or $E = V(\vec{r})$. The points constituting this surface are called the turning points: a name which makes most sense in one dimension. Except for static cases where the turning point is trivially the rest point (and maybe some other weird cases), the particle comes to rest only for an instant at a turning point since the forces are unbalanced there. So it's a place where a particle "ponders for an instant before deciding where to go next". The region with $V > E$ is classically forbidden. Now for most quantum mechanical potential wells, the wave function extends beyond the classical turning point surface into the classical forbidden zone and in fact usually goes to zero only at infinity. If the potential becomes infinite somewhere (which is an idealization of course), the wave function goes to zero: this happens for the infinite square well for instance.

Let's write the 1-dimensional time-independent Schrödinger equation in the form

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{2m}{\hbar^2}(V - E)\psi .$$

- Now solve for ψ for the region with $V > E$ with simplifying the assumption that V is constant in this region.
- Can the solutions be normalized?
- Can the solutions constitute an entire wave function? Can they be part of a wave function? In which regions?
- Although we assumed constant V , what crudely is the behavior of the wave function likely to be like the regions with $V > E$.
- For typical potentials considered at our level, qualitatively what is the likelihood of finding the particle in the classically forbidden region? Why?

002 qfull 01100 3 5 0 tough thinking: 1-d non-degeneracy

15. If there are no internal degrees of freedom (e.g., spin) and no regions of continuous zero wave function (ensured for example by infinite potential barriers), then 1-dimensional stationary states (i.e., energy eigenstates) are non-degenerate. Prove this. Does the proof fail if the stationary states have isolated zeros? What if they have continuous zeros? What happens if there are internal degrees of freedom? **HINTS:** Assume you have two degenerate 1-d stationary states for Hamiltonian H : Ψ_1 and Ψ_2 . Using the eigenproblem equation for each solution, prove that $\Psi_1 \Psi_2' - \Psi_2 \Psi_1'$ equals a constant, that the constant must be zero, and consequently that Ψ_1 and Ψ_2 must be proportional. Consider the case of two isolated infinite square wells: are the stationary states for these well degenerate?

002 qfull 01200 2 3 0 mod math: 3-d exponential wave function, probability

Extra keywords: (Co1-342:6), 3-d wave function, probability, momentum representation

16. Consider the 3-dimensional wave function

$$\Psi(\vec{r}) = A \exp \left[- \sum_i |x_i|/(2a_i) \right] ,$$

where the sum runs over the three Cartesian coordinates and the a_i 's are real positive length parameters.

- a) Calculate the normalization factor A . **HINT:** Recall that the integrand is $|\Psi(\vec{r})|^2 = \Psi(\vec{r})^* \Psi(\vec{r})$. I'm always forgetting this myself when the function is pure real and there is no imaginary part to remind me of it.
- b) Calculate the probability that a measurement of x_i will yield a result between 0 and a_i , where i could be any of the three coordinates. **HINT:** There are no restrictions on values of the other coordinates: they could be anything at all. Thus one just integrates over all of those other coordinate positions remembering normalization of course.
- c) Calculate the probability that simultaneous measurements of x_j and x_k will yield results in the ranges $-a_j$ to a_j and $-a_k$ to a_k , respectively. The j and k could be any pair of the two coordinates. **HINT:** Remember the hint for part (b).
- d) Calculate the probability that a measurement of momentum will yield a result in the element $dp_i dp_j dp_k$ centered at the point $p_i = p_j = 0$, $p_k = \hbar/a_k$. **HINT:** You will need to find the momentum representation of the state.

Chapt. 3 Infinite Square Wells and Other Wells

Multiple-Choice Problems

003 qmult 00050 1 1 1 easy memory: infinite square well

1. In quantum mechanics, the infinite square well can be regarded as the prototype of:
 - a) all bound systems.
 - b) all unbound systems.
 - c) both bound and unbound systems.
 - d) neither bound nor unbound systems.
 - e) Prometheus unbound.

003 qmult 00100 2 4 2 moderate deducto-memory: infinite square well BCs

2. In the infinite square well problem, the wave function and its first spatial derivative are:
 - a) both continuous at the boundaries.
 - b) continuous and discontinuous at the boundaries, respectively.
 - c) both discontinuous at the boundaries.
 - d) discontinuous and continuous at the boundaries, respectively.
 - e) both infinite at the boundaries.

003 qmult 00300 1 1 3 easy memory: boundary conditions

3. Meeting the boundary conditions of quantum mechanical bound systems imposes:
 - a) Heisenberg's uncertainty principle.
 - b) Schrödinger's equation.
 - c) quantization.
 - d) a vector potential.
 - e) a time-dependent potential.

003 qmult 00400 1 1 5 easy memory: continuum of unbound states

4. At energies higher than the bound stationary states there:
 - a) are between one and several tens of unbound states.
 - b) are only two unbound states.
 - c) is a single unbound state.
 - d) are no states.
 - e) is a continuum of unbound states.

003 qmult 00500 1 4 2 easy deducto-memory: tunneling

5. "Let's play *Jeopardy!* For \$100, the answer is: This effect occurs because wave functions can extend (in an exponentially decreasing way albeit) into the classically forbidden region: i.e., the region where a classical particle would have negative kinetic energy."
 - a) What is stimulated radiative emission, Alex?
 - b) What is quantum mechanical tunneling, Alex?
 - c) What is quantization, Alex?

- d) What is symmetrization, Alex?
- e) What is normalization, Alex?

003 qmult 00600 2 1 2 moderate memory: Benzene ring model

6. A simple model of the outer electronic structure of a benzene molecule is a 1-dimensional infinite square well with:
 - a) vanishing boundary conditions.
 - b) periodic boundary conditions.
 - c) aperiodic boundary conditions.
 - d) no boundary conditions.
 - e) incorrect boundary conditions.

Full-Answer Problems

003 qfull 00100 2 3 0 moderate math: infinite square well in 1-d

Extra keywords: infwell

1. You are given the time-independent Schrödinger equation

$$H\psi(x) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E\psi(x)$$

and the infinite square well potential

$$V(x) = \begin{cases} 0, & x \in [0, a]; \\ \infty & \text{otherwise.} \end{cases}$$

- a) What must the wave function be outside of the well in order to satisfy the Schrödinger equation? Why?
- b) What boundary conditions must the wave function satisfy?
- c) Reduce Schrödinger's equation inside the well to the **CLASSICAL** SHO equation with all the constants combined into a wavenumber k .
- d) Solve for the general solution for a single k value. Why can't we allow $E \leq 0$ solutions? Think carefully: it's not because k is imaginary when $E < 0$.
- e) Use the boundary conditions to eliminate some of the solutions with $E > 0$ and to impose quantization on set of solutions. Note physically distinct solutions are indeterminate to within a phase factor $e^{i\phi}$ where ϕ is arbitrary. Give only the general formula and quantization rule for physically distinct solutions.
- f) Normalize the solutions.
- g) Determine the general formula for the eigen-energies.

003 qfull 00400 2 3 0 moderate math: moments of infinite square well

Extra keywords: (Gr-29:2.4)

2. Calculate $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p \rangle$, $\langle p^2 \rangle$, σ_x , and σ_p for the 1-dimensional infinite square well with range $[0, a]$. Recall the general solution is

$$\psi = \sqrt{\frac{2}{a}} \sin(kx) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right),$$

where $n = 1, 2, 3, \dots$. Also check that the Heisenberg uncertainty principle is satisfied.

003 qfull 00500 3 5 0 tough thinking: mixed infwell stationary states

Extra keywords: (Gr-29:2.6)

3. A particle is in a mixed state in a 1-dimensional infinite square well (an infwell) where the well spans $[0, a]$ and the solutions are in the standard form of Gr-26. At time zero the state is

$$\Psi(x, 0) = A [\psi_1(x) + \psi_2(x)] ,$$

where $\psi_1(x)$ and $\psi_2(x)$ are the time-independent 1st and 2nd stationary states of the infwell.

- a) Determine the normalization constant A . Remember the stationary states are orthonormal. Also is the normalization a constant with time? Prove this from the general time evolution equation

$$\frac{d\langle Q \rangle}{dt} = \left\langle \frac{\partial Q}{\partial t} \right\rangle + \frac{1}{\hbar} \langle i[H, Q] \rangle .$$

- b) Now write down $\Psi(x, t)$. Give the argument for why it is the solution. As a simplification in the solution use

$$\omega_1 = \frac{E_1}{\hbar} = \frac{\hbar}{2m} \left(\frac{\pi}{a} \right)^2 ,$$

where E_1 is the ground state energy of the infwell.

- c) Write out $|\Psi(x, t)|^2$ and simplify it so that it is clear that it is pure real. Make use Euler's formula: $e^{ix} = \cos x + i \sin x$. What's different about our mixed state from a stationary state?
- d) Determine $\langle x \rangle$ for the mixed state. Note that the solution is oscillatory. What is the angular frequency ω_q and amplitude of the oscillation. Why would you be wrong if your amplitude was greater than $a/2$.
- e) Determine $\langle p \rangle$ for the mixed state. As Peter Lorre (playing Dr. Einstein—Herman Einstein, Heidelberg 1919) said in *Arsenic and Old Lace* “the quick way, Chonny.”
- f) Determine $\langle H \rangle$ for the mixed state. How does it compare to E_1 and E_2 ?
- g) Say a classical particle had kinetic energy equal to the energy $\langle H \rangle$ found in the part (f) answer. The particle is bounces back and forth between the walls of the infwell. What would its angular frequency be in terms of ω_q and the angular frequency found in the part (d) answer.

003 qfull 01000 3 5 0 tough thinking: 3-d infinite cubical well

Extra keywords: (Gr-124:4.2), separation of Schrödinger equation

4. Consider an infinite cubical well or particle-in-a-box system. The potential is

$$V(x, y, z) = \begin{cases} 0, & \text{for } x, y, \text{ and } z \text{ in the range } 0 \text{ to } a; \\ \infty, & \text{otherwise.} \end{cases}$$

The wave functions must be zero at the boundaries for an infinite well recall.

- a) Solve for the stationary states from the 3-dimensional Schrödinger equation and find their energies in terms of quantum numbers n_x , n_y , and n_z . **HINTS:** Separate the Schrödinger equation into x , y , and z components. Identify the sum of the separation constants as energy or, if you prefer, energy times a constant. Solve separately matching the boundary conditions and then assemble the normalized **TOTAL SOLUTION**. Of course, all three dimensions behave the same so only one of them really needs to be done—which is **NOT** to say that each one is a total solution all by itself.

- b) Is there energy degeneracy? Why?
- c) Determine the 6 lowest energies and their degeneracy? **HINTS:** A systematic approach would be fix an $n_{\max} = \max(n_x, n_y, n_z)$ and count all energies and their degeneracies governed by that n_{\max} . One works one's way up from $n_{\max} = 1$ to as high as one needs to go to encompass the 6 lowest energies. Each n_{\max} governs the energies between $n_{\max}^2 + 2$ and $3n_{\max}^2$ (where we have written the in dimensionless form). Note, e.g., that states described by $(n_x = 4, n_y = 1, n_z = 1)$, $(n_x = 1, n_y = 4, n_z = 1)$, and $(n_x = 1, n_y = 1, n_z = 4)$ are all distinct and degenerate.

003 qfull 01100 1 3 0 easy math: pi-states of a benzene ring

Extra keywords: (Ha-323:2.1)

5. Imagine that we have 6 free electrons in 1-d circular system of radius $r = 1.53 \text{ \AA}$. This system is a simple model of a benzene ring molecule (C_6H_6) of 6 carbon atoms each bonded to a hydrogen (Ke-153). The carbons are bonded by a single-double bond superposition. The free electron system on the benzene constitute the benzene *pi*-states.
- Obtain expressions for the eigenstates, wavenumbers, and eigen-energies of the free electrons. Re-express the wavenumbers and energies in terms of Angstroms and electron-volts. Note $\hbar^2/(2m) = 3.81 \text{ eV-\AA}^2$ for electrons. Sketch the energy level diagram.
 - One electron per carbon lies in the circular state for a benzene ring: these are the π electrons. Assuming that two electrons can be found in any state, what is the total energy of the ground state configurations? **NOTE:** Two electrons can be found in any state because there are two spin states they can be found in. Thus the Pauli exclusion principle is maintained: i.e., only one electron can be found in any single particle state (e.g., Gr-180).
 - What is the energy difference in eV between the lowest empty level and highest occupied level for the ground state configuration? This is the radiation absorption threshold. What is the threshold line wavelength in microns? In what wavelength regime is this line? **NOTE:** The constant $hc = 1.23984 \text{ eV-\mu m}$.
 - Now imagine we broke the benzene ring, but magically kept the length constant. Obtain expressions for the eigenstates, wavenumbers, and eigen-energies of the free electrons. Re-express the wavenumbers and energies in terms of Angstroms and electron-volts. Sketch the energy levels on the previous energy level diagram.
 - What is the ground state energy for the broken ring. What is the change in ground state energy from the unbroken ring. This change is a contribution to the energy required to break the ring or the energy of a resonant π bond.
 - I know we said that somewhere that quantum mechanical bound states always had to have $E > V_{\min}$. But in the ring case we had $V_{\min} = 0$, and we have a state with $E = 0$. So why do we have this paradox? Is the paradox possible in 2 dimensions or 3 dimensions?

Chapt. 4 The Simple Harmonic Oscillator (SHO)

Multiple-Choice Problems

004 qmult 00100 2 4 1 moderate deducto-memory: SHO eigen-energies

1. “Let’s play *Jeopardy!* For \$100, the answer is: $\hbar\omega$.
 - a) What is the energy difference between adjacent simple harmonic oscillator energy levels, Alex?
 - b) What is the energy difference between adjacent infinite square well energy levels, Alex?
 - c) What is the energy difference between most adjacent infinite square well energy levels, Alex?
 - d) What is the energy difference between the first two simple harmonic oscillator energy levels **ONLY**, Alex?
 - e) What is the bar where physicists hang out in Las Vegas, Alex?

Full-Answer Problems

004 qfull 00100 2 3 0 moderate math: SHO ground state analyzed

Extra keywords: (Gr-19:1.14)

1. The simple harmonic oscillator (SHO) ground state is

$$\Psi_0(x, t) = Ae^{-\beta^2 x^2 / 2 - iE_0 t / \hbar} ,$$

where

$$E_0 = \frac{\hbar\omega}{2} \quad \text{and} \quad \beta = \sqrt{\frac{m\omega}{\hbar}} .$$

- a) Verify that the wave function satisfies the full Schrödinger equation for the SHO. Recall that the SHO potential is $V(x) = (1/2)m\omega^2 x^2$.
- b) Determine the normalization constant A .
- c) Calculate the expectation values of x , x^2 , p , and p^2 .
- d) Calculate σ_x and σ_p , and show that they satisfy the Heisenberg uncertainty principle.

004 qfull 00200 2 3 0 moderate thinking: SHO classically forbidden

Extra keywords: (Gr-43:2.15) classical turning points

2. What is the probability of finding a particle in the ground state of a simple harmonic oscillator potential outside of the classically allowed region: i.e., beyond the classical turning points?
HINT: You will have to use a table of the integrated Gaussian function.

004 qfull 00300 2 5 0 moderate thinking: mixed SHO stationary states

Extra keywords: (Gr-43:2.17)

3. A particle in a simple harmonic oscillator (SHO) potential has initial wave function

$$\Psi(x, 0) = A[\psi_0 + \psi_1] ,$$

where A is the normalization constant and the ψ_i are the standard form 0th and 1st SHO eigenstates. Recall the potential is

$$V(x) = \frac{1}{2}m\omega^2 x^2 .$$

Note ω is just an angular frequency parameter of the potential and not **NECESSARILY** the frequency of anything in particular. In the classical oscillator case ω is the frequency of oscillation, of course.

- Determine A assuming it is pure real as we are always free to do.
- Write down $\Psi(x, t)$. There is no need to express the ψ_i explicitly. Why must this $\Psi(x, t)$ be the solution?
- Determine $|\Psi(x, t)|^2$ in simplified form. There should be a sinusoidal function of time in your simplified form.
- Determine $\langle x \rangle$. Note that $\langle x \rangle$ oscillates in time. What is its angular frequency and amplitude.
- Determine $\langle p \rangle$ the quick way using the 1st formula of Ehrenfest's theorem. Check that the 2nd formula of Ehrenfest's theorem holds.

004 qfull 01000 3 5 0 tough thinking: infinite square well/SHO hybrid

Extra keywords: (Mo-424:9.4)

4. Say you have the potential

$$V(x) = \begin{cases} \infty , & x < 0; \\ \frac{1}{2}m\omega^2 x^2 & x \geq 0. \end{cases}$$

- By reflecting on the nature of the potential **AND** on the boundary conditions, identify the set of Schrödinger equation eigenfunctions satisfy this potential. Justify your answer. **HINTS:** Don't try solving the Schrödinger equation directly, just use an already known set of eigenfunctions to identify the new set. This shouldn't take long.
- What is the expression for the eigen-energies of your eigenfunctions?
- What factor must multiply the already-known (and already normalized) eigenfunctions you used to construct the new set you found in part (a) in order to normalize the new eigenfunctions? **HINT:** Use the evenness or oddness (i.e., definite parity) of the already-known set.
- Show that your new eigenfunctions are orthogonal. **HINT:** Use orthogonality and the definite parity of the already-known set.
- Show that your eigenfunctions form a complete set given that the already-known set was complete. **HINTS:** Remember completeness only requires that you can expand any suitably well-behaved function (which means I think it has to be piecewise continuous (Ar-435) and square-integrable (CDL-99) satisfying the same boundary conditions as the set used in the expansion. You don't have to be able to expand any function. Also, use the completeness of the already-known set.

004 qfull 01100 3 5 0 tough thinking: Hermite generating function

5. The generating function method is a powerful technique for getting the properties of the eigenfunctions of Hermitian operators (or self-adjoint operators in math-speak). Orthogonality, the norm value, and the recurrence relations for generating the complete set all fall out with only moderate arduous labor. The only problem is, who the devil thought up the generating function? In the case of Hermite polynomials the generating function—which may or may not have been thought up by Hermite—is

$$g(x, t) = e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H_n \frac{t^n}{n!}$$

(Ar-609ff). The H_n 's are the Hermite polynomials: they are functions of x and n is their order.

- a) Check to see if Hermite did think up “his” generating function at:

<http://www-groups.dcs.st-and.ac.uk/~history/BiogIndex.html>

HINTS: You don't have to do this in a test *mise en scène*.

- b) Show that the two recurrence relations

$$H_{n+1} = 2xH_n - 2nH_{n-1} \quad \text{and} \quad H'_n = 2nH_{n-1}$$

follow by differentiating the generating function with respect to t and x , respectively, and relying on the uniqueness of power series. The recurrence relations provide a means of finding any order of Hermite polynomial. Probably one can efficiently find the coefficients for succeeding orders using an integer arithmetic computer program using the recurrence relation—but that's another (homework) problem.

- c) Use the first recurrence relation to work out and tabulate the polynomials up to 3rd order. You can find the first two polynomials needed to start the process by simple expansion of generating function.
- d) Now for something a bit more challenging. Show that

$$g(x, t) = e^{-t^2 + 2tx} = \sum_{\ell=0}^{\infty} \frac{(-t^2 + 2tx)^\ell}{\ell!} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{k=0}^{[n/2]} \frac{n!}{(n-2k)!k!} (-1)^k (2x)^{n-2k}$$

which implies that

$$H_n = \sum_{k=0}^{[n/2]} \frac{n!}{(n-2k)!k!} (-1)^k (2x)^{n-2k} .$$

Note

$$[n/2] = \begin{cases} n/2 & \text{for } n \text{ even;} \\ (n-1)/2 & \text{for } n \text{ odd.} \end{cases}$$

HINTS: You will have to expand $(-t^2 + 2tx)^n$ in a binomial series and then re-order the summation. A schematic table of the terms ordered in row by ℓ and in column by k makes the re-ordering of the summation clearer: add up diagonals rather than rows.

- e) Prove the following special results from the generating function:

$$H_{2n}(0) = (-1)^n \frac{(2n)!}{n!} , \quad H_{2n+1}(0) = 0 , \quad \text{and} \quad H_n(x) = (-1)^n H_n(-x) .$$

The last results shows that the Hermite polynomials have definite parity: even for n even; odd for n odd.

- f) What is called a Rodrigues formula for the Hermite polynomials can also be derived from the generating function:

$$H_n = (-1)^n e^{x^2} \frac{\partial^n}{\partial x^n} (e^{-x^2}) .$$

Derive this formula. **HINTS:** Write

$$g(x, t) = e^{-t^2+2tx} = e^{x^2} e^{-(t-x)^2}$$

and note that

$$\frac{\partial f(t-x)}{\partial t} = -\frac{\partial f(t-x)}{\partial x} .$$

- g) Hey this question is just going on and on. Now show that Hermite's differential equation

$$H_n'' - 2xH_n' + 2nH_n = 0$$

follows from the two recurrence relations. This result shows that the Hermite polynomials satisfy Hermite's differential equation.

- h) Now consider the Hermite differential equation

$$h'' - 2xh' + 2\nu h = 0 ,$$

where ν is not necessarily an integer ≥ 0 . Try a power series solution

$$h = \sum_{\ell=0}^{\infty} a_{\ell} x^{\ell} ,$$

and show for sufficiently large ℓ and x that the series solutions approximate growing exponentials of the form e^{x^2} and xe^{x^2} —unless ν is a positive or zero integer in which case one gets what kind of solution?

- i) The Hermite differential equation cannot be written in an eigenproblem form with a Hermitian operator since the operator

$$\frac{\partial^2}{\partial x^2} - 2x \frac{\partial}{\partial x}$$

is not in fact Hermitian. I won't ask you to prove this since I don't what to do that myself tonight. But if you substitute for $H_n(x)$ (with n a positive or zero integer) the function

$$\psi_n(x) e^{x^2/2}$$

in the Hermite differential equation, you do an eigenproblem with a Hermitian operator. Find this eigenproblem equation. What are the eigenfunctions and eigenvalues? Are the eigenfunctions square-integrable: i.e., normalizable in a wave function sense? Do the eigenfunctions have definite parity? Are the eigenvalues degenerate for square-integrable solutions? Based on a property of eigenfunctions of a Hermitian operator what can you say about the orthogonality of the eigenfunctions?

- j) In order to normalize the eigenfunctions of part (i) in a wave function sense consider the relation

$$\sum_{m,n=0}^{\infty} \frac{s^m}{m!} \frac{t^n}{n!} e^{-x^2} H_m H_n = e^{-x^2} g(x, s) g(x, t) = e^{-x^2} e^{-s^2+2sx} e^{-t^2+2tx} .$$

Integrate both sides over all x and use uniqueness of power series to find the normalization constants and incidently verify orthogonality.

- k) Now here in part infinity we will make the connection to physics. The simple harmonic oscillator time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial y^2} + \frac{1}{2} m \omega^2 y^2 \psi = E \psi .$$

One can reduce this to the dimensionless eigenproblem of part (i), by changing the variable with

$$x = \beta y .$$

To find β , let

$$A = \frac{\hbar^2}{2m} \quad \text{and} \quad B = \frac{1}{2} m \omega^2$$

and divide equation through by an unknown C , equate what needs to be equated, and solve for C and β . What are the physical solutions and eigen-energies of the SHO eigenproblem?

Chapt. 5 Free Particles and Momentum Representation

Multiple-Choice Problems

005 qmult 00100 1 1 2 easy deducto-memory: definition free particle

1. A free particle is:
 - a) bound.
 - b) unbound.
 - c) both bound and unbound.
 - d) neither bound nor unbound.
 - e) neither here nor there.

005 qmult 00200 1 4 5 easy deducto-mem: free particle case

2. The free particle case (as customarily defined) is when the potential is:
 - a) the simple harmonic oscillator potential (SHO).
 - b) a quasi-SHO potential.
 - c) an infinite square well potential.
 - d) a finite square well potential.
 - e) zero (or a constant) everywhere.

005 qmult 00300 1 4 4 easy deducto-mem: free particle eigenfunction

3. The general expression for the (zero-potential) free particle energy-eigenfunction in 1-dimension is:
 - a) e^{ikx} , where $k = \pm E$.
 - b) e^{kx} , where $k = \pm E$.
 - c) e^{kx} , where $k = \pm\sqrt{2mE}/\hbar$.
 - d) e^{ikx} , where $k = \pm\sqrt{2mE}/\hbar$.
 - e) e^{kx^2} , where $k = \pm\sqrt{2mE}/\hbar$.

005 qmult 00400 1 4 1 easy deducto-mem: free particle normalization

4. The (zero-potential) free particle energy-eigenfunctions cannot represent physical states that a particle can actually be in because they:
 - a) can't be normalized (i.e., they aren't square-integrable).
 - b) can be normalized (i.e., they are square-integrable).
 - c) are growing exponentials.
 - d) don't exist.
 - e) do exist.

005 qmult 00500 1 1 3 easy memory: free particle

5. The free particle stationary states
 - a) can be occupied by a particle.
 - b) can be occupied by two particles.
 - c) cannot actually be occupied by a particle.

- d) are unknown.
- e) are normalizable.

Full-Answer Problems

005 qfull 00100 2 5 0 easy thinking: momentum representation

Extra keywords: (Gr-49:2.21)

1. The initial wave function of a free particle is

$$\Psi(x, 0) = \begin{cases} A, & x \in [-a, a]; \\ 0, & \text{otherwise,} \end{cases}$$

where a and A are positive real numbers. The particle is in a completely zero potential environment: this is usually implied if nothing to the contrary is said.

- a) Determine A from normalization.
- b) Determine $\Psi(k)$ the wavenumber representation of the state of the particle: i.e., the Fourier transform of $\Psi(x, 0)$. Note the wavenumber representation is time-independent: this is because the wavenumber eigenstates are the stationary states of the system. Sketch $\Psi(k)$. Locate the global maximum and the zeros of $\Psi(k)$. Give the expressions for the zero positions.
- c) Determine the wavenumber space probability density $|\Psi(k)|^2$ and show then that $\Psi(k)$ is normalized in wavenumber space. Sketch $|\Psi(k)|^2$ and locate the global maximum and the zeros. Give the expressions for the zero positions.
- d) Crudely estimate and then calculate σ_x , σ_k , and σ_p . Are the results consistent with the Heisenberg uncertainty principle.

005 qfull 00200 3 3 0 tough math: k-representation of half exponential

Extra keywords: (Mo-140:4.4)

2. At time zero, a wave function for a free particle in a zero-potential 1-dimensional space is:

$$\Psi(x, 0) = A e^{-|x|/\ell} e^{ik_0 x}.$$

- a) Determine the normalization constant A . **HINT:** Remember it's $\Psi(x, 0)^* \Psi(x, 0)$ that appears in the normalization equation.
- b) Sketch the x -space probability density $|\Psi(x, 0)|^2$. What is the e -folding distance of the probability density?

NOTE: The e -folding distance is a newish term that means the distance in which an exponential function changes by a factor of e . It can be generalized to any function $f(x)$ using the formula

$$x_e = \left| \frac{f(x)}{f(x)'} \right|,$$

where x_e is the generalized e -folding distance. The generalized e -folding distance is only locally valid to the region near the x where the functions are evaluated. The generalized e -folding distance is also sometimes called the scale height. If $f(x)$ were an exponential function, x_e would be the e -folding distance in the narrow sense. If $f(x)$ were a linear function, x_e would be the distance to the zero of the function.

- c) Show that the wavenumber representation of free particle state is

$$\Psi(k) = \sqrt{\frac{2\ell}{\pi}} \frac{1}{1 + (k_0 - k)^2 \ell^2} .$$

This, of course, is the Fourier transform of $\Psi(x, 0)$. Recall the wavenumber representation is time-independent since the wavenumber eigenstates are the stationary states of the potential.

- d) Confirm that $\Psi(k)$ is normalized in wavenumber space. **HINTS:** You will probably need an integral table—unless you're very, very good. Also remember it's $\Psi(k)^* \Psi(k)$ that appears in the normalization integral; always easy to forget this when dealing with pure real functions.
- e) Write down the time-dependent solution $\Psi(x, t)$ in Fourier transform form? Don't try to evaluate the integral. What is ω in terms of k and energy E ?

005 qfull 00300 3 3 0 tough math: Gaussian free wave packet spreading

Extra keywords: (Gr-50:2.22)

3. A free particle has an initial Gaussian wave function

$$\Psi(x, 0) = Ae^{-ax^2} ,$$

where a and A are real positive constants.

- a) Normalize $\Psi(x, 0)$. **HINT:** Recall that the integrand is $|\Psi(x, t)|^2 = \Psi(x, t)^* \Psi(x, t)$. I'm always forgetting this myself when the function is pure real and there is no imaginary part to remind me of it.
- b) Determine the wavenumber representation $\Psi(k)$ (which is time-independent). This involves a Gaussian integral where you have to complete the square in an exponential exponent. Note

$$\begin{aligned} \exp[-(ax^2 + bx)] &= \exp \left[-a \left(x^2 + \frac{b}{a}x + \frac{b^2}{4a^2} \right) \right] \exp \left(\frac{b^2}{4a} \right) \\ &= \exp \left[-a \left(x + \frac{b}{2a} \right)^2 \right] \exp \left(\frac{b^2}{4a} \right) . \end{aligned}$$

The exponential factor $\exp(b^2/4a)$ comes out of the integral and the integral over the whole x -axis is just a simple Gaussian integral.

- c) Determine $\Psi(x, t)$. You have to again do a Gaussian integral where you have to complete the square in an exponential exponent. It's not that hard to do, but it is tedious and small errors can mess things up.
- d) Find the probability density $|\Psi(x, t)|^2$. This should be a Gaussian if all goes well. Sketch the function and identify the standard deviation σ . What happens to the probability density with time. **HINT:** Note the identities

$$\begin{aligned} \left[\exp \left(\frac{a + ib}{c + id} \right) \right]^* &= \left\{ \exp \left[\frac{ac + i(bc - ad) + bd}{c^2 + d^2} \right] \right\}^* \\ &= \left\{ \exp \left[\frac{ac - i(bc - ad) + bd}{c^2 + d^2} \right] \right\} \\ &= \left[\exp \left(\frac{a - ib}{c - id} \right) \right] \end{aligned}$$

and

$$\left(\sqrt{a+ib}\right)^* = \left(\sqrt{re^{i\phi}}\right)^* = \left(\sqrt{r}e^{i\phi/2}\right)^* = \sqrt{r}e^{-i\phi/2} ,$$

where $a+ib$ magnitude and phase are $r = \sqrt{a^2+b^2}$ and $\phi = \tan^{-1}(b/a)$, respectively.

- e) Find $\langle x \rangle$, $\langle x^2 \rangle$, σ_x , $\langle p \rangle$, $\langle p^2 \rangle$, and σ_p . **HINT:** These results follow immediately from the Gaussian nature of the functions in parts (d) and (b).
- f) Check that the Heisenberg uncertainty principle is satisfied. Does the equality ever hold? What's true about the wave function at the time when the equality holds that is not true at other times?

005 qfull 00400 3 5 0 tough thinking: general free wave packet spreading

Extra keywords: (CDL-342:4)

4. Consider a free particle in one dimension.
 - a) Show using Ehrenfest's theorem that $\langle x \rangle$ is linear in time and that $\langle p \rangle$ is constant.
 - b) Write the equation of motion (time evolution equation) for $\langle p^2 \rangle$, then $\langle [x, p]_+ \rangle$ (the subscript + indicates anticommutator), and then $\langle x^2 \rangle$: i.e., obtain expressions for the time derivatives of these quantities. Simplify the expressions for the derivatives as much as possible, but without loss of generality. You should get nice compact formal results. Integrate these derivatives with respect to time and remember constants of integration.
 - c) Using the results obtained in parts (a) and (b) and for suitable choice of one of the constants of integration, show that

$$(\Delta x^2)(t) = \frac{1}{m^2} (\Delta p^2)_0 t^2 + (\Delta x^2)_0$$

where $(\Delta x^2)_0$ and $(\Delta p^2)_0$ are the initial standard deviations.

005 qfull 00500 3 5 0 tough thinking: x-op and p-op in x and p representation

Extra keywords: (Gr-117:3.51) a very general solution is given

5. In the position representation, the position operator x_{op} is just x , a multiplicative variable. The momentum operator p_{op} in the position representation is

$$p_{\text{dif}} = \frac{\hbar}{i} \frac{\partial}{\partial x} .$$

where we use the subscript "dif" here to indicate explicitly that this is a differentiating operator.

- a) Find the momentum operator p_{op} in the momentum representation. **HINTS:** Operate with p_{dif} on the Fourier transform expansion of a general wave function

$$\Psi(x, t) = \int_{-\infty}^{\infty} \Psi(p, t) \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} dp$$

and work the components of the integral around (using whatever tricks you need) until you have

$$p_{\text{dif}} \Psi(x, t) = \int_{-\infty}^{\infty} f(p, t) \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} dp .$$

The function $f(p, t)$ is the Fourier transform of $p_{\text{dif}} \Psi(x, t)$ and operator acting on $\Psi(p, t)$ to give you $f(p, t)$ is the momentum operator in the momentum representation.

- b) Find the position operator x_{op} in the momentum representation. **HINTS:** The same as for part (a), mutatis mutandis: find the Fourier transform of wave function $x\Psi(x, t)$, etc.

- c) What are the momentum representation versions of x^k and p_{dif}^ℓ ?
- d) What is the momentum representation versions of $x^k p_{\text{dif}}^\ell$ and $p_{\text{dif}}^\ell x^k$. By the by, you should remember how to interpret $x^k p_{\text{dif}}^\ell$ and $p_{\text{dif}}^\ell x^k$: they are two successive operators acting on understood function to the right. Explicitly for a general function $f(x)$, one could write

$$x^k p_{\text{dif}}^\ell f(x) = x^k [p_{\text{dif}}^\ell f(x)]$$

and

$$p_{\text{dif}}^\ell x^k f(x) = p_{\text{dif}}^\ell [x^k f(x)] ,$$

Unfortunately, there is sometimes ambiguity in writing formulae with operators: try to be clear.

- e) What is the momentum representation version of $Q(x, p_{\text{dif}})$ where Q is any linear combination of powers of x and p_{dif} including mixed powers. **HINTS:** Consider the general term

$$\dots x^k p_{\text{dif}}^\ell x^m p_{\text{dif}}^n$$

and figure out what commutes with what.

- f) Show that the expectation value of Q is the same in both representations. **HINT:** Remember the Dirac delta function

$$\delta(k - k') = \int_{-\infty}^{\infty} \frac{e^{i(k-k')x}}{2\pi} dx .$$

Chapt. 6 Foray into Advanced Classical Mechanics

Multiple-Choice Problems

006 qmult 00100 1 1 2 easy memory: Newton's 2nd law

1. Classical mechanics can be very briefly summarized by:
 - a) Newton's *Principia*.
 - b) Newton's 2nd law.
 - c) Lagrange's *Traité de mécanique analytique*.
 - d) Euler's 80 volumes of mathematical works.
 - e) Goldstein 3rd edition.

006 qmult 00200 1 4 1 easy deducto-memory: Lagrangian formulation

Extra keywords: see GPS-12, 17, and 48

2. "Let's play *Jeopardy!* For \$100, the answer is: A formulation of classical mechanics that is usually restricted to systems with holonomic or semi-holonomic virtual-displacement workless constraints without dissipation and uses the function $L = T - V$."
 - a) What is the Lagrangian formulation, Alex?
 - b) What is the Hamiltonian formulation, Alex?
 - c) What is the Leibundgutian formulation, Alex?
 - d) What is the Harrisonian formulation, Alex?
 - e) What is the Sergeant Schultzian formulation, Alex?

006 qmult 00300 1 1 5 easy memory: Hamilton's principle

3. A fruitful starting point for the derivation of Lagrange's equations is:
 - a) Lagrange's lemma.
 - b) Newton's scholium.
 - c) Euler's conjecture.
 - d) Laplace's hypothesis
 - e) Hamilton's principle.

Full-Answer Problems

006 qfull 01000 2 5 0 moderate thinking: Lorentz force

1. The Lorentz force

$$\vec{F} = q \left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B} \right)$$

(here expressed in Gaussian units: Ja-238) can be obtained from Lagrange's equations using a Lagrangian containing a generalized potential

$$U = q \left(\phi - \frac{\vec{v}}{c} \cdot \vec{A} \right) ,$$

where ϕ is the electric potential and \vec{A} is the vector potential of electromagnetism. The Lagrangian is $L = T - U$, where T is the kinetic energy. Lagrange's equations are

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0 ,$$

where q_i is a generalized coordinate (not charge) and \dot{q}_i is the total time derivative of q : (i.e., the rate of change of q_i which describes an actual particle.

Work from the Lorentz force expression for component i to

$$F_i = -\frac{\partial U}{\partial x_i} + \frac{d}{dt} \left(\frac{\partial U}{\partial \dot{x}_i} \right) ,$$

where the x_i are the Cartesian coordinates of a particle (\dot{x}_i are the particle velocity components). Then verify that

$$m\ddot{x}_i = F_i$$

follows from the Lagrange equations.

You may need some hints. Recall that

$$\vec{E} = -\nabla\phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \quad \text{and} \quad \vec{B} = \nabla \times \vec{A}$$

(Ja-219). The Levi-Civita symbol ε_{ijk} will be useful since

$$(\nabla \times A)_i = \varepsilon_{ijk} \frac{\partial}{\partial x_j} A_k .$$

where Einstein summation has been used. Recall

$$\varepsilon_{ijk} = \begin{cases} 1, & ijk \text{ cyclic;} \\ -1, & ijk \text{ anticyclic;} \\ 0, & \text{if two indices the same.} \end{cases}$$

The identity (with Einstein summation)

$$\varepsilon_{ijk}\varepsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$$

is also useful. I've never found an elegant derivation of this last identity: the only proof seems to be by exhaustion. Note also that the total time derivative is interpreted as the rate of change of a quantity as the particle moves. Thus

$$\frac{dA_i}{dt} = \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x_j} \frac{dx_j}{dt} = \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x_j} \dot{x}_j = \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x_j} v_j ,$$

where we again use Einstein summation.

Chapt. 7 Linear Algebra

Multiple-Choice Problems

007 qmult 00100 1 1 5 easy memory: vector addition

1. The sum of two vectors belonging to a vector space is:
 - a) a scalar.
 - b) another vector, but in a different vector space.
 - c) a generalized cosine.
 - d) the Schwarz inequality.
 - e) another vector in the same vector space.

007 qmult 00200 1 4 4 easy deducto-memory: Schwarz inequality

2. "Let's play *Jeopardy!* For \$100, the answer is: $|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$."
 - a) What is the triangle inequality, Alex?
 - b) What is the Heisenberg uncertainty principle, Alex?
 - c) What is Fermat's last theorem, Alex?
 - d) What is the Schwarz inequality, Alex?
 - e) What is Schubert's unfinished last symphony, Alex?

007 qmult 00300 1 4 5 easy deducto-memory: Gram-Schmidt procedure

3. Any set of linearly independent vectors can be orthonormalized by the:
 - a) Pound-Smith procedure.
 - b) Li Po tao.
 - c) Sobolev method.
 - d) Sobolev-P method.
 - e) Gram-Schmidt procedure.

007 qmult 00400 1 4 4 moderate memory: definition unitary matrix

4. A unitary matrix is defined by the expression:
 - a) $U = U^T$, where superscript T means transpose.
 - b) $U = U^\dagger$.
 - c) $U = U^*$.
 - d) $U^{-1} = U^\dagger$
 - e) $U^{-1} = U^*$.

007 qmult 00500 2 3 4 moderate math: trivial eigenvalue problem

5. What are the eigenvalues of

$$\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} ?$$

- a) Both are 0.
- b) 0 and 1.

- c) 0 and -1 .
- d) 0 and 2.
- e) $-i$ and 1.

007 qmult 00600 1 4 5 moderate memory: riddle Hermitian matrix

6. Holy peccant poets Batman, it's the Riddler.

I charge to the right and hit on a ket,
 and if it's not eigen, it's still in the set,
 I charge to left and with a quick draw
 make a new bra from out of a bra.

Not fish nor fowl nor quadratic,
 not uncanny tho oft Q-mechanic,
 and transposed I'm just the right me
 if also complexicated as you can see.

My arrows down drawn from quivered,
 the same when sped to the world delivered
 aside from a steady factor, rock of reality,
 mayhap of a quantum and that's energy.

- a) A unitary operator.
- b) A ket—no, no, a bra vector.
- c) An eigenvalue.
- d) Hamlet.
- e) A Hermitian matrix.

Full-Answer Problems

007 qfull 00090 1 5 0 easy thinking: ordinary vector space

Extra keywords: (Gr-77:3.1)

1. Consider ordinary 3-dimensional vectors with complex components specified by a 3-tuple: (x, y, z) . They constitute a 3-dimensional vector space. Are the following subsets of this vector space vector spaces? If so, what is their dimension? **HINT:** See Gr-76 for all the properties a vector space must have.
 - a) The subset of all vectors all $(x, y, 0)$.
 - b) The subset of all vectors all $(x, y, 1)$.
 - c) The subset of all vectors of the form (a, a, a) , where a is any complex number.

007 qfull 00100 2 5 0 moderate thinking: vector space, polynomial

Extra keywords: (Gr-78:3.2)

2. A vector space is constituted by a set of vectors $\{|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \dots\}$ and a set of scalars $\{a, b, c, \dots\}$ (ordinary complex numbers is all that quantum mechanics requires) subject to two operations vector addition and scalar multiplication obeying the certain rules. Note it is the relations between vectors that make them constitute a vector space. What they “are” we leave general. The rules are:
 - i) A sum of vectors is a vector:

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are any vectors in the space and $|\gamma\rangle$ also in the space. Note we have not defined what vector addition consists of. That definition goes beyond the general requirements.

ii) Vector addition is commutative:

$$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle .$$

iii) Vector addition is associative:

$$(|\alpha\rangle + |\beta\rangle) + |\gamma\rangle = |\alpha\rangle + (|\beta\rangle + |\gamma\rangle) .$$

iv) There is a zero or null vector $|0\rangle$ such that

$$|\alpha\rangle + |0\rangle = |\alpha\rangle ,$$

v) For every vector there is an inverse vector such that

$$|\alpha\rangle + |-\alpha\rangle = |0\rangle .$$

Subtraction of a vector is defined as the addition of its inverse: thus

$$|-\alpha\rangle = -|\alpha\rangle .$$

This is consistent with all ordinary math.

vi) Scalar multiplication of a vector gives a vector:

$$a|\alpha\rangle = |\beta\rangle .$$

vii) Scalar multiplication is distributive on vector addition:

$$a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a(|\beta\rangle) .$$

viii) Scalar multiplication is distributive on scalar addition:

$$(a + b)|\alpha\rangle = a|\alpha\rangle + b|\alpha\rangle .$$

ix) Scalar multiplication is associative with respect to scalar multiplication:

$$(ab)|\alpha\rangle = a(b|\alpha\rangle) .$$

x) One has

$$0|\alpha\rangle = |0\rangle .$$

xi) Finally

$$1|\alpha\rangle = |\alpha\rangle .$$

If any vector in the space can be written as linear combination of a set of linearly independent vectors, that set is called a basis and is said to span the set. The number of vectors in the basis is the dimension of the space. In general there will be infinitely many bases for a space.

Finally the question. Consider the set of polynomials $\{P(x)\}$ (with complex coefficients) and degree less than n . For each of the subsets of this set (specified below) answer the following questions: 1) Is the subset a vector space? 2) If not, what property does it lack? 3) If yes, what is the most obvious basis and what is the dimension of the space?

- a) The subset that is the whole set.
- b) The subset of even polynomials.
- c) The subset where the highest term has coefficient a (i.e., the leading coefficient is a) and a is a general complex number, except $a \neq 0$.
- d) The subset where $P(x = g) = 0$ where g is a general real number.
- e) The subset where $P(x = g) = h$ where g is a general real number and h is a general complex number, except $h \neq 0$.

007 qfull 00110 2 5 0 moderate thinking: unique expansion in basis

Extra keywords: (Gr-78:3.3)

3. Prove that the expansion of a vector in terms of some basis is unique: i.e., the set of expansion coefficients for the vector is unique.

007 qfull 00200 3 5 0 tough thinking: Gram-Schmidt orthonormalization

Extra keywords: (Gr-79:3.4)

4. Say $\{|\alpha_i\rangle\}$ is a basis (i.e., a set of linearly independent vectors that span a vector space), but it is not orthonormal. The first step of the Gram-Schmidt orthogonalization procedure is to normalize the (nominally) first vector to create a new first vector for a new orthonormal basis:

$$|\alpha'_1\rangle = \frac{|\alpha_1\rangle}{||\alpha_1||} ,$$

where recall that the norm of a vector $|\alpha\rangle$ is given by

$$||\alpha|| = || |\alpha_1\rangle || = \sqrt{\langle\alpha|\alpha\rangle} .$$

The second step is create a new second vector that is orthogonal to the new first vector using the old second vector and the new first vector:

$$|\alpha'_2\rangle = \frac{|\alpha_2\rangle - |\alpha'_1\rangle\langle\alpha'_1|\alpha_2\rangle}{|| |\alpha_2\rangle - |\alpha'_1\rangle\langle\alpha'_1|\alpha_2\rangle ||} .$$

Note we have subtracted the projection of $|\alpha_2\rangle$ on $|\alpha'_1\rangle$ from $|\alpha_2\rangle$ and normalized.

- a) Write down the general step of the Gram-Schmidt procedure.
- b) Why must an orthonormal set of non-null vectors be a linearly independent.
- c) Is the result of a Gram-Schmidt procedure independent of the order the original vectors are used? **HINT:** Say you first use vector $|\alpha_a\rangle$ of the old set in the procedure. The first new vector is just $|\alpha_a\rangle$ normalized: i.e., $|\alpha'_a\rangle = |\alpha_a\rangle / ||\alpha_a||$. All the other new vectors will be orthogonal to $|\alpha'_a\rangle$. But what if you started with $|\alpha_b\rangle$ which in general is not orthogonal to $|\alpha_a\rangle$?
- d) How many orthonormalized bases can an n dimensional space have in general? (Ignore the strange $n = 1$ case.) **HINT:** Can't the Gram-Schmidt procedure be started with any vector at all in the vector space?
- e) What happens in the procedure if the original vector set $\{|\alpha_i\rangle\}$ does not, in fact, consist of all linearly independent vectors? To understand this case analyze another apparently

different case. In this other case you start the Gram-Schmidt procedure with n original vectors. Along the way the procedure yields null vectors for the new basis. Nothing can be done with the null vectors: they can't be part of basis or normalized. So you just put those null vectors and the vectors they were meant to replace aside and continue with the procedure. Say you got m null vectors in the procedure and so ended up with $n - m$ non-null orthonormalized vectors. Are these $n - m$ new vectors independent? How many of the old vectors were used in constructing the new $n - m$ non-null vectors and which old vectors were they? Can all the old vectors be reconstructed from the the new $n - m$ non-null vectors? Now answer the original question.

- f) If the original set did consist of n linearly independent vectors, why must the new orthonormal set consist of n linearly independent vectors? **HINT:** Should be just a corollary of the part (e) answer.
- g) Orthonormalize the 3-space basis consisting of

$$|\alpha_1\rangle = \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix}, |\alpha_2\rangle = \begin{pmatrix} i \\ 3 \\ 1 \end{pmatrix}, \quad \text{and} \quad |\alpha_3\rangle = \begin{pmatrix} 0 \\ 32 \\ 0 \end{pmatrix}.$$

Input the vectors into the procedure in the reverse of their nominal order: why might a marker insist on this? Note setting kets equal to columns is a lousy notation, but you-all know what I mean. The bras, of course, should be "equated" to the row vectors. **HINT:** Make sure you use the normalized new vectors in the construction procedure.

007 qfull 00300 2 3 0 moderate math: prove the Schwarz inequality

Extra keywords: (Gr-80:3.5)

5. As Andy Rooney says (or used to say if this problem has reached the stage where only old fogys remember that king of the old fogys) don't you just hate magic proofs where you start from some unmotivated expression and do a number of unmotivated steps to arrive at result that you could never have been guessed from the way you were going about getting it. Well let's see if we can prove the Schwarz inequality

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$$

sans too many absurd steps. Note the equality only holds in two cases. First when $|\beta\rangle = a|\alpha\rangle$, where a is some complex constant. Second, when either or both of $|\alpha\rangle$ and $|\beta\rangle$ are null vectors: in this case one has zero equals zero.

- a) First consider two vectors $|\alpha\rangle$ and $|\beta\rangle$ which are completely general, except that $|\alpha\rangle$ is not a null vector. Because $|\alpha\rangle$ is not null, it can be normalized. Let $|\hat{\alpha}\rangle = |\alpha\rangle/||\alpha||$ be the normalized version of $|\alpha\rangle$. Now determine $|\beta_{||}\rangle$, the component of $|\beta\rangle$ in the $|\alpha\rangle$ direction and the norm squared of $|\beta_{||}\rangle$.

Note that for vector space

$$|\gamma\rangle + |0\rangle = |\gamma\rangle,$$

where $|0\rangle$ is the null vector and $|\gamma\rangle$ is general. For an inner product vector space, this rule implies for general vector $|\delta\rangle$ that

$$\langle\delta|\gamma\rangle + \langle\delta|0\rangle = \langle\delta|\gamma\rangle,$$

and thus that

$$\langle\delta|0\rangle = 0 = \langle 0|\delta\rangle.$$

- b) Now what is $|\beta_{\perp}\rangle$, the component of $|\beta\rangle$ that is everything other than $|\beta_{||}\rangle$.

- c) What basic inner product vector space requirement must the norm squared of $|\beta_{\perp}\rangle$ satisfy? What does this requirement then imply about the relationship between the norms squared of $|\beta\rangle$ and $|\beta_{\parallel}\rangle$?
- d) From the part (c) answer the Schwarz inequality should now follow.
- e) Does the Schwarz inequality hold if $|\alpha\rangle$ is a null vector?

007 qfull 00310 1 3 0 easy math: find a generalized angle

Extra keywords: (Gr-80:3.6)

6. The general inner-product vector space definition of generalized angle according to Gr-79 is

$$\cos \theta_{\text{gen}} = \frac{|\langle \alpha | \beta \rangle|}{\sqrt{\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle}} ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are general non-zero vectors.

- a) Is this definition completely consistent with the ordinary definition of an angle from the ordinary vector dot product? Why not?
- b) Find the generalized angle between vectors

$$|\alpha\rangle = \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix} \quad \text{and} \quad |\beta\rangle = \begin{pmatrix} 4-i \\ 0 \\ 2-2i \end{pmatrix} .$$

007 qfull 00400 1 3 0 easy math: prove triangle inequality

Extra keywords: (Gr-80:3.7)

7. Prove the triangle inequality:

$$|| |\alpha\rangle + |\beta\rangle || \leq ||\alpha|| + ||\beta|| .$$

HINT: Start with $|| |\alpha\rangle + |\beta\rangle ||^2$, expand, and use reality and the Schwarz inequality.

007 qfull 00500 3 3 0 tough math: simple matrix identities

Extra keywords: (Gr-87:3.12)

8. Prove the following matrix identities:

- a) $(AB)^T = B^T A^T$, where superscript “T” means transpose.
- b) $(AB)^\dagger = B^\dagger A^\dagger$, where superscript \dagger means Hermitian conjugate.
- c) $(AB)^{-1} = B^{-1} A^{-1}$.
- d) $(UV)^{-1} = (UV)^\dagger$ (i.e., UV is unitary) given that U and V are unitary. In other words, prove the product of unitary matrices is unitary.
- e) $(AB)^\dagger = AB$ (i.e., AB is Hermitian) given that A and B are commuting Hermitian matrices. Does the converse hold: i.e., does $(AB)^\dagger = AB$ imply A and B are commuting Hermitian matrices? **HINTS:** Find a trivial counterexample. Try $B = A^{-1}$.
- f) $(A+B)^\dagger = A+B$ (i.e., $A+B$ is Hermitian) given that A and B are Hermitian. Does the converse hold? **HINT:** Find a trivial counterexample to the converse.
- g) $(U+V)^\dagger = (U+V)^{-1}$ (i.e., $U+V$ is unitary) given that U and V are unitary—that is, prove this relation if it’s indeed true—if it’s not true, prove that it’s not true. **HINT:** Find a simple counterexample: e.g., two 2×2 unit matrices.

 007 qfull 00510 2 5 0 moderate thinking: commuting operations
Extra keywords: (Gr-84)

9. There are 4 simple operations that can be done to a matrix: inverting, (-1) , complex conjugating $(*)$, transposing (T) , and Hermitian conjugating (\dagger) . Prove that all these operations mutually commute. Do this systematically: there are

$$\binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$$

combinations of the 2 operations. We assume the matrices have inverses for the proofs involving them.

 007 qfull 00600 3 3 0 tough math: basis change results
Extra keywords: (Gr-87:3.14)

10. Do the following.
- Prove that matrix multiplication is preserved under similarity or linear basis change: i.e., if $A_e B_e = C_e$ in the e -basis, then $A_f B_f = C_f$ in the f -basis where S is the basis change matrix from e -basis to the f -basis. Basis change does not in general preserve symmetry, reality, or Hermiticity. But since I don't want to find the counterexamples, I won't ask you to.
 - If H_e in the e -basis is a Hermitian matrix and the basis change to the f -basis U is unitary, prove that H_f is Hermitian: i.e., Hermiticity is preserved.
 - Prove that basis orthonormality is preserved through a basis change U iff (if and only if) U is unitary.

 007 qfull 00700 2 5 0 moderate thinking: square-integrable, inner product
Extra keywords: no analog Griffiths' problem, but he discusses this case on Gr-96

11. If $f(x)$ and $g(x)$ are square-integrable complex functions, then the inner product

$$\langle f|g \rangle = \int_{-\infty}^{\infty} f^* g \, dx$$

exists: i.e., is convergent to a finite value. In other words, that $f(x)$ and $g(x)$ are square-integrable is sufficient for the inner product's existence.

- a) Prove the statement for the case where $f(x)$ and $g(x)$ are real functions. **HINT:** In doing this it helps to define a function

$$h(x) = \begin{cases} f(x) & \text{where } |f(x)| \geq |g(x)| \text{ (which can be called } f \text{ region);} \\ g(x) & \text{where } |f(x)| < |g(x)| \text{ (which can be called the } g \text{ region),} \end{cases}$$

and show that it must be square-integrable. Then "squeeze" $\langle f|g \rangle$.

- b) Now prove the statement for complex $f(x)$ and $g(x)$. **HINTS:** Rewrite the functions in terms of their real and imaginary parts: i.e.,

$$f(x) = f_{\text{Re}}(x) + i f_{\text{Im}}(x)$$

and

$$g(x) = g_{\text{Re}}(x) + i g_{\text{Im}}(x) .$$

Now expand

$$\langle f|g \rangle = \int_{-\infty}^{\infty} f^* g \, dx$$

in the terms of the new real and imaginary parts and reduce the problem to the part (a) problem.

- c) Now for the easy part. Prove the converse of the statement is false. **HINT:** Find some trivial counterexample.
- d) Now another easy part. Say you have a vector space of functions. Prove the following two statements are equivalent: 1) the inner product property holds; 2) the functions are square-integrable.

007 qfull 00800 2 3 0 moderate math: Gram-Schmidt, Legendre polynomials

Extra keywords: (Gr-96:3.25)

12. Using the Gram-Schmidt procedure, orthonormalize the set of polynomial vectors 1, x , and x^2 on the interval $[-1, 1]$. Compare these to the Legendre polynomials $\{P_n(x)\}$ which are orthogonal on the interval $[-1, 1]$, but not normalized. The normalized Legendre polynomials are given by

$$P_{n \text{ normalized}}(x) = \sqrt{n + \frac{1}{2}} P_n(x) ,$$

where $P_n(x)$ is a standard Legendre polynomial (e.g., Ar-547).

Table: Legendre Polynomials

Order n	P_n
0	$P_0 = 1$
1	$P_1 = x$
2	$P_2 = \frac{1}{2}(3x^2 - 1)$
3	$P_3 = \frac{1}{2}(5x^3 - 3x)$
4	$P_4 = \frac{1}{8}(35x^4 - 30x^2 + 3)$
5	$P_5 = \frac{1}{8}(63x^5 - 70x^3 + 15x)$

Note—The reason why the Legendre polynomials aren't normalized is that the standard forms are what one gets straight from the generating function. The generating function approach to the Legendre polynomials allows you to prove many of their properties quickly (e.g., Ar-534).

007 qfull 00900 1 3 0 easy math: verifying a sinusoidal basis

Extra keywords: (Gr-96:3.26)

13. Consider the set of trigonometric functions defined by

$$f(x) = \sum_{n=0}^N [a_n \sin(nx) + b_n \cos(nx)]$$

on the interval $[-\pi, \pi]$. Show that the functions defined by

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} , \quad \text{where} \quad k = 0, \pm 1, \pm 2, \dots, \pm N$$

are an orthonormal basis for the trigonometric set. What is the dimension of the space spanned by the basis?

007 qfull 01000 2 3 0 moderate math: reduced SHO operator, Hermiticity

Extra keywords: (Gr-99:3.28), dimensionless simple harmonic oscillator Hamiltonian

14. Consider the operator

$$Q = -\frac{d^2}{dx^2} + x^2 .$$

- a) Show that $f(x) = e^{-x^2/2}$ is an eigenfunction of Q and determine its eigenvalue.
 b) Under what conditions, if any, is Q a Hermitian operator? **HINTS:** Recall

$$\langle g|Q^\dagger|f\rangle^* = \langle f|Q|g\rangle$$

is the defining relation for the Hermitian conjugate Q^\dagger of operator Q . You will have to write the matrix element $\langle f|Q|g\rangle$ in the position representation and use integration by parts to find the conditions.

007 qfull 01100 2 5 0 moderate thinking: Hilbert space problems

Extra keywords: (Gr-103:3.33)

15. Do the following.

- a) Show explicitly that any linear combination of two functions in the Hilbert space $L_2(a, b)$ is also in $L_2(a, b)$. (By explicitly, I mean don't just refer to the definition of a vector space which, of course requires the sum of any two vectors to be a vector.)
 b) For what values of real number s is $f(x) = |x|^s$ in $L_2(-a, a)$
 c) Show that $f(x) = e^{-|x|}$ is in $L_2 = L_2(-\infty, \infty)$. Find the wavenumber space representation of $f(x)$: recall the wavenumber "orthonormal" basis states in the position representation are

$$\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}} .$$

007 qfull 01200 2 5 0 moderate thinking: Hermitian conjugate of AB

16. Some general operator and vector identities should be proven.

- a) Prove that the bra corresponding to vector $Q|\beta\rangle$ is $\langle\beta|Q^\dagger$ for Q and $|\beta\rangle$ general. **HINT:** Define $|\beta'\rangle = Q|\beta\rangle$ and then take the inner product of that vector with another general vector $|\alpha\rangle$ and use the definition of the Hermitian conjugate. I'd use bra $\langle\beta'|$ on ket $|\alpha\rangle$ and then reverse the order complex conjugating.
 b) Show that the Hermitian conjugate of a scalar c is just its complex conjugate.
 c) Prove for operators, not matrices, that

$$(AB)^\dagger = B^\dagger A^\dagger .$$

The result is, of course, consistent with matrix representations of these operators. But there are representations in which the operators are not matrices: e.g., the momentum operator in the position representation is differentiating operator

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} .$$

Our proof holds for such operators too since we done the proof in the general operator-vector formalism.

007 qfull 01300 3 5 0 tough thinking: operators and matrices isomorphism

17. Expressions involving vector linear transformations or operators often (always?) isomorphic to the corresponding matrix expressions when the operators are represented by matrices in particular orthonormal bases. We would like to demonstrate this statement for a few important simple cases. For clarity express operators with hats (e.g., \hat{A}) and leave the corresponding matrices unadorned (e.g., A). Consider a general orthonormal basis $\{|i\rangle\}$ where i serves as a labeling index. Recall that the unit operator using this basis is

$$I = |i\rangle\langle i| ,$$

where we use the Einstein summation rule, and so there is a sum on i . Recall that the ij th matrix element of A is defined by

$$A_{ij} = \langle i | \hat{A} | j \rangle .$$

This definition means that the scalar product $\langle a | \hat{A} | b \rangle$, where $|a\rangle$ and $|b\rangle$ are general vectors, can be reexpressed by matrix expression:

$$\langle a | \hat{A} | b \rangle = \langle a | i \rangle \langle i | \hat{A} | j \rangle \langle j | b \rangle = a_i^* A_{ij} b_j = \vec{a}^\dagger A \vec{b} ,$$

where \vec{a} and \vec{b} are column vector n-tuples and where we have used the Einstein rule.

Prove that the following operator expressions are isomorphic to their corresponding matrix expressions.

- a) Sum of operators $\hat{A} + \hat{B}$.
- b) Product of operators $\hat{A}\hat{B}$.
- c) Hermitian conjugation \hat{A}^\dagger .
- d) The identity $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$.

007 qfull 01400 2 5 0 moderate thinking: bra ket projector completeness

Extra keywords: (Gr-118:3.57) See also CDL-115, 138

18. For an inner product vector space there is some rule for calculating the inner product of two general vectors: an inner product being a complex scalar. If $|\alpha\rangle$ and $|\beta\rangle$ are general vectors, then their inner product is denoted by

$$\langle \alpha | \beta \rangle ,$$

where in general the order is significant. Obviously different rules can be imagined for a vector space which would lead to different values for the inner products. But the rule must have three basic properties:

- (1) $\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^* ,$
- (2) $\langle \alpha | \alpha \rangle \geq 0 ,$ where $\langle \alpha | \alpha \rangle = 0$ if and only if $|\alpha\rangle = |0\rangle$,

and

- (3) $\langle \alpha | (b|\beta\rangle + c|\gamma\rangle) = b\langle \alpha | \beta \rangle + c\langle \alpha | \gamma \rangle ,$

where $|\alpha\rangle$, $|\beta\rangle$, and $|\gamma\rangle$ are general vectors of the vector space and b and c are general complex scalars.

There are some immediate corollaries of the properties. First, if $\langle \alpha | \beta \rangle$ is pure real, then

$$\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle .$$

Second, if $\langle \alpha | \beta \rangle$ is pure imaginary, then

$$\langle \beta | \alpha \rangle = -\langle \alpha | \beta \rangle .$$

Third, if

$$|\delta\rangle = b|\beta\rangle + c|\gamma\rangle ,$$

then

$$\langle \delta | \alpha \rangle^* = \langle \alpha | \delta \rangle = b\langle \alpha | \beta \rangle + c\langle \alpha | \gamma \rangle$$

which implies

$$\langle \delta | \alpha \rangle = b^* \langle \beta | \alpha \rangle + c^* \langle \gamma | \alpha \rangle .$$

This last result makes

$$\left(\langle \beta | b^* + \langle \gamma | c^* \right) | \alpha \rangle = b^* \langle \beta | \alpha \rangle + c^* \langle \gamma | \alpha \rangle$$

a meaningful expression. The 3rd rule for a vector product inner space and last corollary together mean that the distribution of inner product multiplication over addition happens in the normal way one is used to.

Dirac had the happy idea of defining dual space vectors with the notation $\langle \alpha |$ for the dual vector of $|\alpha\rangle$: $\langle \alpha |$ being called the bra vector or bra corresponding to $|\alpha\rangle$, the ket vector or ket: “bra” and “ket” coming from “bracket.” Mathematically, the bra $\langle \alpha |$ is a linear function of the vectors. It has the property of acting on a general vector $|\beta\rangle$ and yielding a complex scalar: the scalar being exactly the inner product $\langle \alpha | \beta \rangle$.

One immediate consequence of the bra definition can be drawn. Let $|\alpha\rangle$, $|\beta\rangle$, and a be general and let

$$|\alpha'\rangle = a|\alpha\rangle .$$

Then

$$\langle \alpha' | \beta \rangle = \langle \beta | \alpha' \rangle^* = a^* \langle \beta | \alpha \rangle^* = a^* \langle \alpha | \beta \rangle$$

implies that the bra corresponding to $|\alpha'\rangle$ is given by

$$\langle \alpha' | = a^* \langle \alpha | = \langle \alpha | a^* .$$

The use of bra vectors is perhaps unnecessary, but they do allow some operations and properties of inner product vector spaces to be written compactly and intelligibly. Let's consider a few nice uses.

- a) The projection operator or projector on to unit vector $|e\rangle$ is defined by

$$P_{\text{op}} = |e\rangle \langle e| .$$

This operator has the property of changing a vector into a new vector that is $|e\rangle$ times a scalar. It is perfectly reasonable to call this new vector the component of the original vector in the direction of $|e\rangle$: this definition of component agrees with our 3-dimensional Euclidean definition of a vector component, and so is a sensible generalization of that the 3-dimensional Euclidean definition. This generalized component would also be the contribution of a basis of which $|e\rangle$ is a member to the expansion of the original vector: again the usage of the word component is entirely reasonable. In symbols

$$P_{\text{op}} |\alpha\rangle = |e\rangle \langle e | \alpha \rangle = a |e\rangle ,$$

where $a = \langle e | \alpha \rangle$.

Show that $P_{\text{op}}^2 = P_{\text{op}}$, and then that $P_{\text{op}}^n = P_{\text{op}}$, where n is any integer greater than or equal to 1. **HINTS:** Write out the operators explicitly and remember $|e\rangle$ is a unit vector.

- b) Say we have

$$P_{\text{op}} |\alpha\rangle = a |\alpha\rangle ,$$

where $P_{\text{op}} = |e\rangle \langle e|$ is the projection operator on unit vector $|e\rangle$ and $|\alpha\rangle$ is unknown non-null vector. Solve for the **TWO** solutions for a . Then solve for the $|\alpha\rangle$ vectors corresponding to these solutions. **HINTS:** Act on both sides of the equation with $\langle e|$ to find an equation for one a value. This equation won't yield the 2nd a value—and that's the hint for finding the 2nd a value. Substitute the a values back into the original equation to determine the corresponding $|\alpha\rangle$ vectors. Note one a value has a vast degeneracy in general: i.e., many vectors satisfy the original equation with that a value.

- c) The Hermitian conjugate of an operator Q is written Q^\dagger . The definition of Q^\dagger is given by the expression

$$\langle \beta | Q^\dagger | \alpha \rangle = \langle \alpha | Q | \beta \rangle^* ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are general vectors. Prove that the bra corresponding to ket $Q|\beta\rangle$ must be $\langle \beta | Q^\dagger$ for general $|\alpha\rangle$. **HINTS:** Let $|\beta'\rangle = Q|\beta\rangle$ and substitute this for $Q|\beta\rangle$ in the defining equation of the Hermitian conjugate operator. Note operators are not matrices (although they can be represented as matrices in particular bases), and so you are not free to use purely matrix concepts: in particular the concepts of transpose and complex conjugation of operators are not generally meaningful.

- d) Say we define a particular operator Q by

$$Q = |\phi\rangle\langle\psi| ,$$

where $|\phi\rangle$ and $|\psi\rangle$ are general vectors. Solve for Q^\dagger . Under what condition is

$$Q^\dagger = Q ?$$

When an operator equals its Hermitian conjugate, the operator is called Hermitian just as in the case of matrices.

- e) Say $\{|e_i\rangle\}$ is an orthonormal basis. Show that

$$|e_i\rangle\langle e_i| = \mathbf{1} ,$$

where we have used Einstein summation and $\mathbf{1}$ is the unit operator. **HINT:** Expand a general vector $|\alpha\rangle$ in the basis.

Chapt. 8 Operators, Hermitian Operators, Bracket Formalism

Multiple-Choice Problems

008 qmult 00090 1 4 5 easy deducto-memory: example Hilbert space

1. “Let’s play *Jeopardy!* For \$100, the answer is: A space of all square-integrable functions on the x interval (a, b) .”
 - a) What is a non-inner product vector space, Alex?
 - b) What is a non-vector space, Alex?
 - c) What is a Dilbert space, Alex?
 - d) What is a Dogbert space, Alex?
 - e) What is a Hilbert space, Alex?

008 qmult 00100 1 1 3 easy memory: complex conjugate of scalar product

2. The scalar product $\langle f|g \rangle^*$ in general equals:
 - a) $\langle f|g \rangle$.
 - b) $i\langle f|g \rangle$.
 - c) $\langle g|f \rangle$.
 - d) $\langle f|i|g \rangle$.
 - e) $\langle f|(-i)|g \rangle$.

008 qmult 00200 1 4 3 easy deducto-memory: what operators do

3. “Let’s play *Jeopardy!* For \$100, the answer is: It changes a vector into another vector.”
 - a) What is a wave function, Alex?
 - b) What is a scalar product, Alex?
 - c) What is an operator, Alex?
 - d) What is a bra, Alex?
 - e) What is a telephone operator, Alex?

008 qmult 00300 2 1 5 moderate memory: Hermitian conjugate of product

4. Given general operators A and B , $(AB)^\dagger$ equals:
 - a) AB .
 - b) $A^\dagger B^\dagger$.
 - c) A .
 - d) B .
 - e) $B^\dagger A^\dagger$.

008 qmult 00400 2 5 5 moderate thinking: general Hermitian conjugation

5. The Hermitian conjugate of the operator $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A$ (with λ a scalar and A an operator) is:
 - a) $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A$.
 - b) $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A^\dagger$.
 - c) $A|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda^*$.
 - d) $A|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda$.

e) $A^\dagger|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda^*$.

008 qmult 00500 1 1 5 easy memory: compatible observables

6. Compatible observables:

- a) anticommute.
- b) are warm and cuddly with each other.
- c) have no hair.
- d) have no complete simultaneous orthonormal basis.
- e) commute.

008 qmult 00600 1 1 3 easy memory: parity operator

7. The parity operator Π acting on $f(x)$ gives:

- a) df/dx .
- b) $1/f(x)$.
- c) $f(-x)$.
- d) 0.
- e) a spherical harmonic.

008 qmult 00700 1 4 3 easy deducto-memory: braket expectation value

8. Given the position representation for an expectation value

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi(x)^* Q \Psi(x) dx ,$$

what is the braket representation?

- a) $\langle Q | \Psi^* | Q \rangle$.
- b) $\langle \Psi^* | Q | \Psi \rangle$.
- c) $\langle \Psi | Q | \Psi \rangle$.
- d) $\langle \Psi | Q^\dagger | \Psi \rangle$.
- e) $\langle Q | \Psi | Q \rangle$.

008 qmult 00800 1 4 3 easy deducto-memory: Hermitian eigenproblem

9. What are the three main properties of the solutions to a Hermitian operator eigenproblem?

- a) (i) The eigenvalues are pure **IMAGINARY**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors **DO NOT** span all space.
- b) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space in **ALL** cases.
- c) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space for **ALL FINITE-DIMENSIONAL** spaces. In infinite dimensional cases they may or may not span all space.
- d) (i) The eigenvalues are pure **IMAGINARY**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space in **ALL FINITE-DIMENSIONAL** spaces. In infinite dimensional cases they may or may not span all space.
- e) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized.

008 qmult 00900 1 4 5 easy deducto-memory: definition observable

10. “Let’s play *Jeopardy!* For \$100, the answer is: A physically significant Hermitian operator possessing a complete set of eigenvectors.”
- What is Hermitian conjugate, Alex?
 - What is a bra, Alex?
 - What is a ket, Alex?
 - What is an inobservable, Alex?
 - What is an observable, Alex?

008 qmult 01000 1 4 4 easy deducto-memory: time-energy inequality

11. In the precisely-formulated time-energy inequality the Δt is:
- the standard deviation of time.
 - the standard deviation of energy.
 - a Hermitian operator.
 - the characteristic time for an observable’s value to change by one standard deviation.
 - the characteristic time for the system to do nothing.

Full-Answer Problems

008 qfull 00010 1 1 0 easy memory: what is a ket?

- What is a ket (representative general symbol $|\Psi\rangle$)?

008 qfull 00015 1 1 0 easy memory: what is a bra?

- What is a bra? (Representative general symbol $\langle\Psi|$.)

008 qfull 00020 1 1 0 easy memory: why the bracket formalism?

- Why is quantum mechanics at the advanced level formulated in the bracket formalism?

008 qfull 00030 2 5 0 moderate thinking: Hermiticity and expectation values

Extra keywords: (Gr-94:3.21)

- For T to be a Hermitian operator one requires that $T^\dagger = T$. Recall the definition of Hermitian conjugate for a general operator Q is

$$\langle\alpha|Q^\dagger|\beta\rangle = \langle\beta|Q|\alpha\rangle^* ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are general vectors.

- Prove if T is Hermitian, that expectation value of a general vector $|\alpha\rangle$,

$$\langle\gamma|T|\gamma\rangle ,$$

is pure real.

- Prove if the expectation value

$$\langle\gamma|T|\gamma\rangle$$

is always pure real for general $|\gamma\rangle$, that T is Hermitian. This is the converse of the statement in part (a). **HINT:** Let $|\alpha\rangle$ and $|\beta\rangle$ be general and construct a $|\xi\rangle = |\alpha\rangle + c|\beta\rangle$, where c is a general complex scalar. Expand both sides of

$$\langle\xi|T|\xi\rangle = \langle\xi|T^\dagger|\xi\rangle^* = \langle\xi|T^\dagger|\xi\rangle ,$$

use the condition that all expectation values are pure real, and construct two equations that must both hold: one for $c = 1$ and one for $c = i$. Solve the two equations.

- What simple statement follows from the proofs in parts (a) and (b)?

 008 qfull 00040 2 3 0 moderate math: solving an eigenproblem

Extra keywords: (Gr-94:3.22) also diagonalizing a matrix.

5. Consider

$$T = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix}.$$

- a) Is T Hermitian?
- b) Solve for the eigenvalues. Are they real?
- c) Determine the normalized eigenvectors. Since eigenvectors are not unique to within a phase factor, the marker insists that you arrange your eigenvectors so that the first component of each is 1. Are they orthogonal?
- d) Using the eigenvectors as columns construct the inverse of a unitary matrix transformation which applied to T gives a diagonalized version of T . Find this diagonalized version T^d . What is special about the diagonal elements?
- e) Compare the determinant $\det|T|$, trace $\text{Tr}(T)$, and eigenvalues of T to those of T^d .

 008 qfull 00500 2 5 0 moderate thinking: x-op in general formalism

Extra keywords: and k-op and p-op in general formalism too

6. The general formalism of quantum mechanics requires states to be vectors in Hilbert spaces and dynamical variables to be governed or determined (choose your verb) by observables (Hermitian operators with complete sets of eigenstates: i.e., sets that form a basis for the Hilbert space). These requirements are a Procrustian bed for the position, wavenumber (or momentum), and kinetic energy operators. These operators have complete sets of eigenvectors in a sense, but those eigenvectors aren't in any Hilbert space, because they can't be normalized. Nevertheless everything works out consistently if some identifications are made. The momentum and kinetic energy eigenstates are the same as the wavenumber eigenstates, and so we won't worry about them. The momentum and kinetic energy eigenvalues are different, of course.

NOTE: Procrustes (he who stretches) was a robber (or cannibal) with a remarkable bed that fit all guests—by racking or hacking according to whether small or tall. Theseus fit Procrustes to his own bed—and this was before that unfortunate incident with the Minotaur.

- a) Consider the x_{op} eigenproblem in the general form

$$x_{\text{op}}|x\rangle = x|x\rangle,$$

where x is the eigenvalue and $|x\rangle$ is the eigenvector. The eigenvalues x and eigenvectors $|x\rangle$'s form continuous, not discrete, sets. The unity operator for the x_{op} basis is therefore

$$\mathbf{1} = \int dx |x\rangle\langle x|,$$

where it is implied that the integral is over all space. An ideal measurement of position yields x and, by quantum mechanical postulate, puts the system in state $|x\rangle$. But the system can't be really be in an unnormalizable state which is what the $|x\rangle$'s turn out to be. The system can be in an integral linear combination of such states.

Expand a general state $|\Psi\rangle$ in the x_{op} basis and identify what $|\Psi\rangle$ is in the position representation. Then identify what the inner product of two x_{op} eigenvectors $\langle x'|x\rangle$ must be. Why can't the $|x\rangle$ be in the Hilbert space? What is the position representation of $|x\rangle$? Prove that x_{op} in the position operator is just x itself.

- b) Repeat part (a), mutatis mutandis, for k_{op} .

- c) What must $\langle x|k \rangle$ be? This is just an identification, not a proof—there are no proofs. **HINT:** Expand $|\Psi\rangle$ in the wavenumber representation and then operate on $|\Psi\rangle$ with $\langle x|$.
- d) What is $\langle k|k' \rangle$ if we insert the position representation unit operator given the answer to part (c).
- e) In order to have consistency with past work what must the matrix elements $\langle x|k_{\text{op}}|x \rangle$, $\langle x|H_{\text{op}}|x \rangle$, and $\langle k|x_{\text{op}}|k \rangle$ be. Note these are just identifications, not proofs—there are no proofs. We omit $\langle k|H_{\text{op}}|k \rangle$ —you're not ready for $\langle k|H_{\text{op}}|k \rangle$ as Jack Nicholson would snarl—if he were teaching intro quantum.

008 qfull 00100 2 5 0 moderate thinking: expectation values two ways

Extra keywords: (Gr-108:3.35)

7. Consider the observable Q and the general **NORMALIZED** vector $|\Psi\rangle$. By quantum mechanics postulate, the expectation of Q^n , where $n \geq 0$ is some integer, for $|\Psi\rangle$ is

$$\langle Q^n \rangle = \langle \Psi | Q^n | \Psi \rangle .$$

- a) Assume Q has a discrete spectrum of eigenvalues q_i and orthonormal eigenvectors $|q_i\rangle$. It follows from the general probabilistic interpretation postulate of quantum mechanics, that expectation value of Q^n for $|\Psi\rangle$ is given by

$$\langle Q^n \rangle = \sum_i q_i^n |\langle q_i | \Psi \rangle|^2 .$$

Show that this expression for $\langle Q^n \rangle$ also follows from the one in the preamble. What is $\sum_i |\langle q_i | \Psi \rangle|^2$ equal to?

- b) Assume Q has a continuous spectrum of eigenvalues q and Dirac-orthonormal eigenvectors $|q\rangle$. (Dirac-orthonormal means that $\langle q' | q \rangle = \delta(q' - q)$, where $\delta(q' - q)$ is the Dirac delta function. The term Dirac-orthonormal is all my own invention: it needed to be.) It follows from the general probabilistic interpretation postulate of quantum mechanics, that expectation value of Q^n for $|\Psi\rangle$ is given by

$$\langle Q^n \rangle = \int dq q^n |\langle q | \Psi \rangle|^2 .$$

Show that this expression for $\langle Q^n \rangle$ also follows from the one in the preamble. What is $\int dq |\langle q | \Psi \rangle|^2$ equal to?

008 qfull 00200 2 5 0 moderate thinking: simple commutator identities

8. Prove the following commutator identities.

- a) $[A, B] = -[B, A]$.
- b) $\left[\sum_i a_i A_i, \sum_j b_j B_j \right] = \sum_{ij} a_i b_j [A_i, B_j]$, where the a_i 's and b_j 's are just complex numbers.
- c) $[A, BC] = [A, B]C + B[A, C]$.
- d) $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$. This has always seemed to me to be perfectly useless however true.
- e) $(c[A, B])^\dagger = c^* [B^\dagger, A^\dagger]$, where c is a complex number.
- f) The special case of the part (e) identity when A and B are Hermitian and c is pure imaginary. Is the operator in this special case Hermitian or anti-Hermitian?

 008 qfull 00300 3 5 0 tough thinking: nontrivial commutator identities

Extra keywords: (Gr-111:3.41) but considerably extended.

9. Prove the following somewhat more difficult commutator identities.

a) Given

$$[B, [A, B]] = 0, \quad \text{prove} \quad [A, F(B)] = [A, B]F'(B),$$

where A and B are general operators aside from the given condition and $F(B)$ is a general operator function of B . **HINTS:** Proof by induction is probably best. Recall that any function of an operator is (or is that should be) expandable in a power series of the operator: i.e.,

$$F(B) = \sum_{n=0}^{\infty} f_n B^n,$$

where f_n are constants.

b) $[x, p] = i\hbar$.

c) $[x, p^n] = i\hbar n p^{n-1}$. **HINT:** Recall the part (a) answer.

d) $[p, x^n] = -i\hbar n x^{n-1}$. **HINT:** Recall the part (a) answer.

 008 qfull 01400 3 5 0 tough thinking: general uncertainty principle

10. You have a strange looking operator:

$$\ell = \frac{\delta Q}{\Delta Q} + i \frac{\delta R}{\Delta R}.$$

where Q and R are general Hermitian operators, ΔQ and ΔR are the standard deviations of Q and R , and

$$\delta Q \equiv Q - \langle Q \rangle \quad \text{and} \quad \delta R \equiv R - \langle R \rangle.$$

(a) Write down the Hermitian conjugate ℓ^\dagger .

(b) Show $\ell^\dagger \ell$ a Hermitian operator and that it is a positive definite operator: i.e., that $\langle \ell^\dagger \ell \rangle \geq 0$. **HINT:** If you have to think about these results for more than a few seconds, then just assume them and go on.

(c) Multiply out $\ell^\dagger \ell$ and gather the cross terms into a commutator operator. Substitute for δQ and δR in the commutator using their definitions and simplify it.

(d) Evaluate the expectation value of the multiplied out $\ell^\dagger \ell$ operator. Simplify it remembering the definition of standard deviation.

(e) Remembering the positive definite result from part (b), find an inequality satisfied by $\Delta Q \Delta R$.

(f) Since the whole of the foregoing mysterious procedure could have been done with Q and R interchanged in the definition of ℓ , what second inequality must be satisfied by $\Delta Q \Delta R$.

(g) What third $\Delta Q \Delta R$ inequality is implied by two previous ones.

 008 qfull 01500 2 3 0 moderate math: x-H uncertainty relation

Extra keywords: (Gr-110:3.39)

11. Answer the following questions.

a) What is the uncertainty relation for operators x and H ? Work it out until the expectation value is for the momentum operator p .

- b) What is the time-dependent expression for any observable expectation value $\langle Q \rangle = \langle \Psi(t) | Q | \Psi(t) \rangle$ when the state $|\Psi(t)\rangle$ is expanded in the discrete set of stationary states (i.e., energy eigenstates) with their time-dependent factors included to allow for the time dependence of $|\Psi(t)\rangle$. Let the set of stationary states with explicit time dependence be $\{e^{-iE_j t/\hbar} |\phi_j\rangle\}$. Note functions of t commute with observables: observables may depend on time, but they don't contain time derivatives.
- c) If state $|\Psi(t)\rangle$ from part (b) is itself the stationary state $e^{-iE_j t/\hbar} |\phi_j\rangle$, what the expectation value? Is the expectation value time independent?
- d) Derive the special form of the uncertainty relation for operators x and H for the case of a stationary state of H ? What in fact is σ_H for a stationary state? **HINT:** Remember Ehrenfest's theorem.

008 qfull 01600 3 5 0 tough thinking: neutrino oscillation

Extra keywords: (Gr-120:3.58)

12. There are systems that exist apart from 3-dimensional Euclidean space: they are internal degrees of freedom such intrinsic spin of an electron or the proton-neutron identity of a nucleon (isospin: see, e.g., En-162 or Ga-429). Consider such an internal system for which we can only detect two states:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

This internal system is 2-dimensional in the abstract vector sense of dimensional: i.e., it can be described completely by an orthonormal basis of consisting of the 2 vectors we have just given. When we measure this system we force it into one or other of these states: i.e., we make the fundamental perturbation. But the system can exist in a general state of course:

$$|\Psi(t)\rangle = c_+(t)|+\rangle + c_-(t)|-\rangle = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} .$$

- a) Given that $|\Psi(t)\rangle$ is **NORMALIZED** what equation must the coefficients $c_+(t)$ and $c_-(t)$ satisfy. **HINT:** I don't want Schrödinger's equation as an answer.
- b) For reasons only known to Mother Nature, the states we can measure (eigenvectors of whatever operator they may be) $|+\rangle$ and $|-\rangle$ are **NOT** eigenstates of the Hamiltonian that governs the time evolution of internal system. Let the Hamiltonian's eigenstates (i.e., the stationary states) be $|+\prime\rangle$ and $|-\prime\rangle$: i.e.,

$$H|+\prime\rangle = E_+|+\prime\rangle \quad \text{and} \quad H|-\prime\rangle = E_-|-\prime\rangle ,$$

where E_+ and E_- are the eigen-energies. Verify that the general state $|\Psi(t)\rangle$ expanded in these energy eigenstates,

$$|\Psi(t)\rangle = c_+ e^{-iE_+ t/\hbar} |+\prime\rangle + c_- e^{-iE_- t/\hbar} |-\prime\rangle$$

satisfies the general vector form of the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle .$$

HINT: This requires a one-line answer.

- c) The Hamiltonian for this internal system has no differential operator form since there is no wave function. The matrix form in the $|+\rangle$ and $|-\rangle$ representation is

$$H = \begin{pmatrix} f & g \\ g & f \end{pmatrix} .$$

Given that H is Hermitian, prove that f and g must be real.

- d) Solve for the eigenvalues (i.e., eigen-energies) of Hamiltonian H and for its normalized eigenvectors $|+\rangle$ and $|-\rangle$ in column vector form.
- e) Given at $t = 0$ that

$$|\Psi(0)\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

show that

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}(a+b)e^{-i(f+g)t/\hbar}|+\rangle + \frac{1}{\sqrt{2}}(a-b)e^{-i(f-g)t/\hbar}|-\rangle$$

and then show that

$$|\Psi(t)\rangle = e^{-ift/\hbar} \left[a \begin{pmatrix} \cos(gt/\hbar) \\ -i \sin(gt/\hbar) \end{pmatrix} + b \begin{pmatrix} -i \sin(gt/\hbar) \\ \cos(gt/\hbar) \end{pmatrix} \right].$$

HINT: Recall the time-zero coefficients of expansion in basis $\{|\phi_i\rangle\}$ are given by $\langle\phi_i|\Psi(0)\rangle$.

- f) For the state found given the part (e) question, what is the probability at any time t of measuring (i.e., forcing by the fundamental perturbation) the system into state

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}?$$

HINT: Note a and b are in general complex.

- g) Set $a = 1$ and $b = 0$ in the probability expression found in the part (f) answer. What is the probability of measuring the system in state $|+\rangle$? in state $|-\rangle$? What is the system doing between the two states?

NOTE: The weird kind of oscillation between detectable states we have discussed is a simple model of neutrino oscillation. Just as an example, the detectable states could be the electron neutrino and muon neutrino and the particle oscillates between them. Really there are three flavors of neutrinos and a three-way oscillation may occur. There is growing evidence that neutrino oscillation does happen. (This note may be somewhat outdated due to that growth of evidence.)

Chapt. 9 Time Evolution

Multiple-Choice Problems

009 qmult 00100 1 4 1 moderate deducto-memory: constant of the motion

1. What are the conditions for observable Q to be a constant of the motion.
 - a) $[H, Q] = 0$ and $\partial Q/\partial t = 0$.
 - b) $[H, Q] \neq 0$ and $\partial Q/\partial t \neq 0$.
 - c) $[H, Q] > 0$ and $\partial Q/\partial t > 0$.
 - d) $[H, Q] < 0$ and $\partial Q/\partial t < 0$.
 - e) $[H, Q] \geq 0$ and $\partial Q/\partial t \geq 0$.

Full-Answer Problems

009 qfull 00100 3 5 0 tough thinking: time evolution, virial theorem

Extra keywords: (Gr-117:3.53)

1. Answer the following questions *On the road to the Virial Theorem* (starring Bing Crosby, Bob Hope, and Dorothy Lamour). **HINTS:** The answers to the earlier parts help answering the later parts. But you can still answer some later parts even if you don't get all the earlier parts.

- a) Given that $e^{-iE_nt/\hbar}|\phi_n\rangle$, a stationary state (i.e., an eigen-energy state) of a time-independent Hamiltonian with its time-dependence factor explicitly shown, show that the expectation value for this state of any time-independent operator A is a constant with respect to time: i.e.,

$$\frac{d\langle A \rangle}{dt} = 0 .$$

HINT: This is easy.

- b) Given that $|\phi_n\rangle$ is a stationary state of H and A is a general operator, show that

$$\langle \phi_n | [H, A] | \phi_n \rangle = 0 .$$

HINT: This is easy.

- c) Prove that $[A, BC] = [A, B]C + B[A, C]$ for general operators A , B , and C .
- d) Prove $[x, p] = i\hbar$.
- e) Prove that

$$[H, x] = -\frac{i\hbar}{m}p .$$

- f) Prove that

$$[H, p] = i\hbar \left(\frac{\partial V}{\partial x} \right) .$$

g) Starting general time evolution equation (or general equation of motion)

$$\frac{d\langle Q \rangle}{dt} = \left\langle \frac{\partial Q}{\partial t} \right\rangle + \frac{1}{\hbar} \langle i[H, Q] \rangle$$

show that

$$\frac{d\langle xp \rangle}{dt} = 2\langle T \rangle - \left\langle x \frac{\partial V}{\partial x} \right\rangle ,$$

where $T = p^2/(2m)$ is the kinetic energy operator.

h) Show that

$$\frac{d\langle xp \rangle}{dt} = \frac{d\langle px \rangle}{dt} .$$

HINT: This is easy.

i) Now for a **STATIONARY STATE** prove the 1-d virial theorem:

$$\langle T \rangle_{\text{stationary}} = \frac{1}{2} \left\langle x \frac{\partial V}{\partial x} \right\rangle_{\text{stationary}} .$$

HINT: Don't forget part (a) and what the general equation of motion says.

j) Given potential $V(x) \propto x^\lambda$, show that the virial theorem reduces to

$$\langle T \rangle_{\text{stationary}} = \frac{\lambda}{2} \langle V \rangle_{\text{stationary}} .$$

Chapt. 10 Measurement

Multiple-Choice Problems

010 qmult 00100 1 1 1 easy memory: fundamental perturbation

1. In an ideal quantum mechanical measurement of an observable A :
 - a) the measurement always detects an **EIGENVALUE** of the observable and projects the system into an **EIGENSTATE** of the observable corresponding to that eigenvalue.
 - b) the measurement always detects an **EXPECTATION VALUE** of the observable and projects the system into an **EIGENSTATE** of the observable.
 - c) the measurement always detects an **EXPECTATION VALUE** of the observable and projects the system into an **NON-EIGENSTATE** of the observable.
 - d) the measurement always detects an **3 EIGENVALUES** of the observable and projects the system into an **NON-EIGENSTATE** of the observable.
 - e) The measurement always detects an **EXPECTATION VALUE** of the observable and projects the system into a **STATIONARY STATE**.

Full-Answer Problems

Chapt. 11 The Central Force Problem and Orbital Angular Momentum

Multiple-Choice Problems

011 qmult 00100 1 4 3 easy deducto-memory: central force

1. In a central force problem the force depends only on:
 - a) the angle of the particle.
 - b) the vector \vec{r} from the center to the particle.
 - c) the radial distance r from the center to the particle.
 - d) the magnetic quantum number of the particle.
 - e) the uncertainty principle.

011 qmult 00200 1 1 2 easy memory: separation of variables

2. The usual approach to getting the eigenfunctions of the Hamiltonian in multi-dimensions is:
 - a) non-separation of variables.
 - b) separation of variables.
 - c) separation of invariables.
 - d) non-separation of invariables.
 - e) non-separation of variables/invariables.

011 qmult 00300 1 4 2 easy deducto-memory: relative/cm reduction

3. "Let's play *Jeopardy!* For \$100, the answer is: By writing the two-body Schrödinger equation in relative/center-of-mass coordinates."
 - a) How do you reduce a **ONE-BODY** problem to a **TWO-BODY** problem, Alex?
 - b) How do you reduce a **TWO-BODY** problem to a **ONE-BODY** problem, Alex?
 - c) How do you solve a one-dimensional infinite square well problem, Alex?
 - d) How do you solve for the simple harmonic oscillator eigenvalues, Alex?
 - e) How do you reduce a **TWO-BODY** problem to a **TWO-BODY** problem, Alex?

011 qmult 00310 1 4 4 easy deducto-memory: reduced mass

4. The formula for the reduced mass m for two-body system (with bodies labeled 1 and 2) is:
 - a) $m = m_1 m_2$.
 - b) $m = 1/m_1 m_2$.
 - c) $m = (m_1 + m_2)/m_1 m_2$.
 - d) $m = m_1 m_2/(m_1 + m_2)$.
 - e) $m = 1/m_1$.

011 qmult 00400 1 4 2 easy deducto memory: spherical harmonics

5. The eigensolutions of the angular part of the Hamiltonian for the central force problem are:
 - a) the linear harmonics.
 - b) the spherical harmonics.
 - c) the square harmonics.

- d) the Pythagorean harmonics.
- e) the Galilean harmonics.

011 qmult 00500 1 4 3 easy deducto memory: spherical harmonic Y_{00}

6. Just about the only spherical harmonic that people remember—and they really should remember it too—is $Y_{00} =$:
- a) $e^{im\phi}$.
 - b) r^2 .
 - c) $1/\sqrt{4\pi}$.
 - d) θ^2 .
 - e) $2a^{-3/2}e^{-r/a}$.

011 qmult 00900 1 4 3 easy deducto-memory: s electrons

7. “Let’s play *Jeopardy!* For \$100, the answer is: What the $\ell = 0$ electrons (or zero orbital angular momentum electrons) are called in spectroscopic notation.”
- a) What are the Hermitian conjugates, Alex?
 - b) What Herman’s Hermits, Alex?
 - c) What are s electrons, Alex?
 - d) What are p electrons, Alex?
 - e) What are h electrons, Alex?

011 qmult 01000 1 4 2 easy deducto-memory: spdf designations

8. Conventionally, the spherical harmonic eigenstates for angular momentum quantum numbers

$$\ell = 0, 1, 2, 3, 4, \dots$$

are designated by:

- a) a, b, c, d, e , etc.
- b) s, p, d, f , and then alphabetically following f : i.e., g, h , etc.
- c) x, y, z, xx, yy, zz, xxx , etc.
- d) A, C, B, D, E, etc.
- e) \$@%&*!!

Full-Answer Problems

011 qfull 00090 2 5 0 moderate thinking: 2-body reduced to 1-body problem

Extra keywords: (Gr-178:5.1)

1. The 2-body time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m_1}\nabla_1^2\psi - \frac{\hbar^2}{2m_2}\nabla_2^2\psi + V\psi = E_{\text{total}}\psi.$$

If the V depends only on $\vec{r} = \vec{r}_2 - \vec{r}_1$ (the relative vector), then the problem can be separate into two problems: a relative problem 1-body equivalent problem and a center-of-mass 1-body equivalent problem. The center of mass vector is

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{M},$$

where $M = m_1 + m_2$.

- a) Determine the expressions for \vec{r}_1 and \vec{r}_2 in terms of \vec{R} and \vec{r} .
- b) Determine the expressions for ∇_1^2 and ∇_2^2 in terms of ∇_{cm}^2 (the center-of-mass Laplacian operator) and ∇^2 (the relative Laplacian operator). Then re-express kinetic operator

$$-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2$$

in terms of ∇_{cm}^2 and ∇^2 . **HINTS:** The x , y , and z direction components of vectors can all be treated separately and identically since X and x depend only on x_1 and x_2 , etc. You can introduce a reduced mass to make the transformed kinetic energy operator simpler.

- c) Now separate the 2-body Schrödinger equation assuming $V = V(\vec{r})$. What are the solutions of the center-of-mass problem? How would you interpret the solutions of the relative problem? **HINT:** I'm only looking for a short answer to the interpretation question.

011 qfull 00100 2 3 0 moderate math: solving the azimuthal component

Extra keywords: solving the azimuthal component of the central force problem

2. In the central force problem the separated azimuthal part of the Schrödinger equation is:

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi(\phi) ,$$

where $-m^2$ is the constant of separation for the azimuthal part. The constant has been parameterized in terms of m (which is not mass) since it turns out that for normalizable (and therefore physically allowed) solutions that m must be an integer. The m quantity is the z -component angular momentum quantum number or magnetic quantum number (MEL-59). The latter name arises since the z -components of the angular momentum manifest themselves most noticeably in magnetic field phenomena.

- a) Solve for the $\Phi(\phi)$ solutions. Why can we rule out complex m ? **HINT:** Use an exponential trial function.
- b) Impose the condition that the solutions be single-valued for all physically distinct azimuthal angles in order to obtain the allowed values of m . Note this condition, although seemingly very natural, cannot be justified just from considering the azimuthal solution alone since physically we only need that $|\Phi(\phi)|^2$ be single-valued for physically distinct azimuthal angles. The requirement that polar angle solutions be normalizable (i.e., square-integrable) implies that the $\Phi(\phi)$ solutions be single-valued. The justification is given by, e.g., Griffiths (see Gr-126–127).
- c) Normalize the allowed $\Phi(\phi)$ solutions. Note the $\Phi(\phi)$ solutions are in fact conventionally left unnormalized: i.e., the coefficient of the special function that is the solution is left as just 1. Normalization is conventionally imposed on the total angular solution.
- d) Show that $\Phi(\phi)$ solutions are also eigenfunctions of the z -component of the angular momentum:

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi} .$$

What are the eigenvalues?

011 qfull 01000 3 5 0 tough thinking: the nearly rigid rotator

3. You have a 3-dimensional system consisting of two non-identical particles of masses m_1 and m_2 . The two particles form a nearly rigid rotator. The relative time-independent Schrödinger equation for the system is:

$$\left[-\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{L^2}{2\mu r^2} + V(r) \right] \Psi(r, \theta, \phi) = E \Psi(r, \theta, \phi) ,$$

where r , θ , and ϕ are the relative coordinates, $\mu = m_1 m_2 / (m_1 + m_2)$ is the reduced mass, and the potential is

$$V(r) = \begin{cases} 0, & \text{for } r \in [a - \Delta a/2, a + \Delta a/2]; \\ \infty, & \text{otherwise.} \end{cases}$$

- a) Assume that Δa is so much smaller than a that $L^2/(2\mu r^2) \approx L^2/(2\mu a^2)$. Now separate the equation into radial and angular parts using E_{rad} and E_{rot} as the respective separation constants: $E_{\text{rad}} + E_{\text{rot}} = E$. Let the radial solutions be $R(r)$. You know what the angular solutions should be. Write down the separated equations.
- b) For the radial equation assume that r varies so much more slowly than R over the region of non-infinite potential that

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) \approx \frac{\partial^2 R}{\partial r^2}$$

in that region. Change the coordinate variable to $x = r - (a - \Delta a/2)$ for simplicity: the non-infinite region of the potential then is then the x range $[0, \Delta a]$. With this approximation solve for the radial eigenstates and eigen-energies. Normalize the eigenstates. **HINTS:** Holy *déjà vu* all over again Batman, it's the 1-dimensional infinite square well problem. Don't mix up a and Δa .

- c) Write down the eigenstates (just their general symbol, not expressions) and eigen-energy expression for the rotational equation. What is the degeneracy of each eigen-energy? **HINTS:** You shouldn't be trying to solve the equation. You should know what the eigenstates are.
- d) Write the general expression for the total wave function. How many quantum numbers does it depend on?
- e) Write down the general expression for the total energy. Which causes a greater change in energy: a change of 1 in the quantum number controlling the radial energy or a change of 1 in the quantum number controlling the rotational energy? Remember $\Delta a \ll a$ by assumption.
- f) Sketch the energy level diagram.

Chapt. 12 The Hydrogenic Atom

Multiple-Choice Problems

012 qmult 00050 1 1 1 easy memory: hydrogen atom, 2-body

1. The hydrogen atom is the simplest of all neutral atoms because:
 - a) it is a 2-body system.
 - b) it is a 3-body system.
 - c) it has no electrons.
 - d) it has many electrons.
 - e) it is the most abundant element in the universe.

012 qmult 00100 1 1 3 easy memory: radial wave function requirements

2. What basic requirements must a radial function meet in order to be a physical radial wave function?
 - a) Satisfy the radial part of the Schrödinger equation and grow exponentially as $r \rightarrow \infty$.
 - b) Not satisfy the radial part of the Schrödinger equation and grow exponentially as $r \rightarrow \infty$.
 - c) Satisfy the radial part of the Schrödinger equation and be normalizable.
 - d) Not satisfy the radial part of the Schrödinger equation and be normalizable.
 - e) None at all.

012 qmult 00190 1 1 2 easy memory: hydrogen wave functions

3. The hydrogen wave functions contain a factor that causes them to:
 - a) increase exponentially with radius.
 - b) decrease exponentially with radius.
 - c) increase logarithmically with radius.
 - d) increase quadratically with radius.
 - e) increase linearly with wavelength.

012 qmult 00200 1 4 1 easy deducto-memory: associated Laguerre polyn.

4. What special functions are factors in the radial equation of the hydrogenic atom?
 - a) The associated Laguerre polynomials.
 - b) The unassociated Laguerre polynomials.
 - c) The associated jaguar polynomials.
 - d) The unassociated jaguar polynomials.
 - e) The Hermite polynomials.

012 qmult 01000 1 4 1 easy deducto-memory: atomic spectroscopy

5. Almost all would agree that the most important empirical means for learning about atomic energy eigenstates is:
 - a) spectroscopy.
 - b) microscopy.
 - c) telescopy.

- d) pathology.
- e) astrology.

Full-Answer Problems

012 qfull 00100 1 1 0 easy memory: separation of two body problem.

1. The full Schrödinger equation for the hydrogenic atom is a function of two positions, one for the electron and one for the nucleus. What must one do to turn the problem into a central force problem for one body?

012 qfull 00200 2 5 0 moderate thinking: how does $\langle r \rangle$ vary with n ?

2. How does the mean radius (expectation value radius) $\langle r \rangle_{nlm}$ for the hydrogenic atom vary with increasing n (i.e., with increasing energy)?

012 qfull 00300 2 1 0 moderate memory: H atom quantum numbers

3. What are the 3 quantum numbers of the hydrogenic atom derived from the spatial Schrödinger equation?

012 qfull 00400 2 1 0 moderate memory: s electron polar plot

4. Sketch the polar plot for an s electron (i.e., an $\ell = 0$ electron)?

012 qfull 00500 2 5 0 moderate thinking: rotating or standing wave functions

5. Are the hydrogenic wave functions Ψ_{nlm} rotating wave or standing wave functions?

012 qfull 00600 2 5 0 moderate thinking: rotating or standing wave functions

6. Can there be hydrogenic atom stationary-state standing wave functions?

012 qfull 00700 2 5 0 moderate thinking: what is the Bohr magneton?

7. What is the Bohr magneton?

012 qfull 00800 2 5 0 moderate thinking: atomic magnetic moments

8. Why should an atom have a magnetic moment?

012 qfull 00900 1 3 0 easy math: first 4 Laguerre polynomials keyword first 4 Laguerre polynomials, Rodrigues' formula

9. Using Rodrigues' formula for Laguerre polynomials (**NOT** Legendre polynomials) determine the first 4 Laguerre polynomials.

012 qfull 01000 3 3 0 tough thinking : separation of external potential

Extra keywords: separation of external potential, 1st order expansion

10. Consider the initial hydrogenic-atom Schrödinger equation where the position variables are still for the nucleus and electron. Say we add perturbation potentials $V_n(\vec{r}_n)$ for the nucleus and $V_e(\vec{r}_e)$ for the electron. We further specify that these perturbation potentials vary only linearly with position. How would one have to treat these potentials in order to transform to the center-of-mass/relative coordinate system and separate the Schrödinger equation? **HINTS:** Have you heard of the Taylor's series? You'll have to express the \vec{r}_n and \vec{r}_e in terms of relative and center of mass coordinates.

012 qfull 01200 2 3 0 moderate math: s electron in nucleus

Extra keywords: (Gr-142:4.14)

11. Let's consider the probability that the electron of a hydrogenic atom in the ground state will be in the nucleus. Recall the wave function for ground state is

$$\Psi_{100}(\vec{r}) = R_{10}(r)Y_{00}(\theta, \phi) = 2a^{-3/2}e^{-r/a} \times \frac{1}{\sqrt{4\pi}},$$

where $a = a_{\text{Bohr}}/Z$: $a_{\text{Bohr}} \approx 0.529\text{\AA}$ is the Bohr radius and Z is the nuclear charge.

- a) First assume that the wave function is accurate down to $r = 0$. It actually can't be of course. The wave function was derived assuming a point nucleus and the nucleus is in fact extended. However, the extension of the nucleus is of order 10^5 times smaller than the Bohr radius, and so the effect of a finite nucleus is a small perturbation. Given that the nuclear radius is b , calculate the probability of finding the electron in the nucleus. Use $\epsilon = 2b/a$ to simplify the formula. **HINT:** The formula

$$g(n, x) = \int_0^x e^{-t} t^n dt = n! \left(1 - e^{-x} \sum_{\ell=0}^n \frac{x^\ell}{\ell!} \right)$$

could be of use.

- b) Expand the part (a) answer in ϵ power series and show to lowest non-zero order that

$$P(r < b, \epsilon \ll 1) = \frac{1}{6}\epsilon^3 = \frac{4}{3} \left(\frac{b}{a} \right)^3.$$

- c) An alternate approach to find the probability of the electron being in the nucleus is assume $\Psi(\vec{r})$ can be approximated by $\Psi(0)$ over nucleus. Thus

$$P(r < b) \approx \left(\frac{4\pi}{3} \right) b^3 |\Psi(0)|^2.$$

Is this result consistent with the part (b) answer?

- d) Assume $b \approx 10^{-15}\text{m}$ and $a = 0.5 \times 10^{-10}\text{m}$. What is the approximate numerical value for finding the electron in the nucleus? You can't interpret this result as "the fraction of the time the electron spends in the nucleus." Nothing in quantum mechanics tells us that the electron spends time definitely anywhere. One should simply stop with what quantum mechanics gives: the result is the probability of finding the electron in nucleus.

012 qfull 01300 3 5 0 tough thinking: derivation of quantum \vec{J} current

Extra keywords: derivation of quantum \vec{J} current, correspondence principle

12. Let's see if we can derive the probability current density from the correspondence principle. Note that the classical current density is given by $\vec{j}_{\text{cl}} = \vec{v}_{\text{cl}}\rho_{\text{cl}}$. (a) First off we have to figure out what the quantum mechanical ρ and \vec{j} are classified as in quantum mechanics? Are they operators or wave functions or expectation values or are they just their own things? Well they may indeed be just their own things, but one can interpret them as belonging to one of the three mentioned categories. Which? (b) Well now that part (a) is done we can use the correspondence principle to find an operator corresponding to classical \vec{j}_{cl} . What are the appropriate operators to replace the classical ρ_{cl} and \vec{v}_{cl} with (i.e., how are ρ_{cl} and \vec{v}_{cl} quantized)? (c) Have you remembered the quantization symmetrization rule? (d) Now go to it and derive the quantum mechanical \vec{j} . You might find the 3-d integration-by-parts rule handy:

$$\int_V \Psi \nabla \chi dV = \int_A \Psi \chi d\vec{A} - \int_V \nabla \Psi \chi dV,$$

where \int_V is for integral over all volume V and \int_A is for integral over all vectorized surface area of volume V .

Chapt. 13 General Theory of Angular Momentum

Multiple-Choice Problems

013 qmult 00100 1 1 4 easy memory: ang. mom. commutation relations

1. The fundamental angular momentum commutation relation and a key corollary are, respectively:

- a) $[J_i, J_j] = 0$ and $[J^2, J_i] = J_i$.
- b) $[J_i, J_j] = J_k$ and $[J^2, J_i] = 0$.
- c) $[J_i, J_j] = 0$ and $[J^2, J_i] = 0$.
- d) $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$ and $[J^2, J_i] = 0$.
- e) $[x_i, p_j] = i\hbar\delta_{ij}$, $[x_i, x_j] = 0$, and $[p_i, p_j] = 0$.

013 qmult 01000 1 1 5 easy memory: rigid rotator eigen-energies

2. For a rigid rotator the rotational eigen-energies are proportional to:

- a) $\ell\hbar$.
- b) $\ell^2\hbar^2$.
- c) $\hbar^2/[\ell(\ell+1)]$.
- d) \hbar^2/ℓ^2 .
- e) $\ell(\ell+1)\hbar^2$.

Full-Answer Problems

013 qfull 00090 2 5 0 moderate math: kroneckar delta, Levi-Civita

1. There are two symbols that are very useful in dealing with quantum mechanical angular momentum and in many other contexts in physics: the Kroneckar delta:

$$\delta_{ij} = \begin{cases} 1, & i = j; \\ 0, & i \neq j; \end{cases}$$

and the Levi-Civita symbol

$$\varepsilon_{ijk} = \begin{cases} 1, & \text{if } ijk \text{ is a cyclic permutation of } 123 \text{ (3 cases);} \\ -1, & \text{if } ijk \text{ is an anticyclic permutation of } 123 \text{ (3 cases);} \\ 0, & \text{if any two indices are the same.} \end{cases}$$

NOTE: Leopold Kroneckar (1823–1891) was a German mathematician although born in what is now Poland. Tullio Levi-Civita (1873–1941) was an Italian mathematician: the “C” in Civita is pronounced “ch”.

- a) Prove $\delta_{ij}\delta_{ik} = \delta_{jk}$, where we are using Einstein summation here and below, of course.
- b) Now the toughie. Prove

$$\varepsilon_{ijk}\varepsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}.$$

HINTS: I know of no simple one or two line proof. The best I've ever thought of was to consider cases where $jkm\ell$ span 3, 1, and 2 distinct values and to show that the two expressions are equal in all cases.

c) Now the cinchy one. Prove

$$\varepsilon_{ijk}\varepsilon_{ijm} = 2\delta_{km} .$$

d) What does $\varepsilon_{ijk}\varepsilon_{ijk}$ equal? Note there is Einstein summation on all indices now.

013 qfull 00100 2 5 0 moderate thinking: angular momentum operator identities

2. Prove the following angular momentum operator identities. **HINT:** Recall the fundamental angular momentum commutator identities:

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k \quad \text{and} \quad [J^2, J_i] = 0 ,$$

and the definition

$$J_{\pm} \equiv J_x \pm iJ_y .$$

a) $[J^2, J_{\pm}] = 0$.

b) $[J_z, J_{\pm}] = \pm\hbar J_{\pm}$.

c) $J_{\pm}^{\dagger}J_{\pm} = J_{\mp}J_{\pm} = J^2 - J_z(J_z \pm \hbar)$.

d)

$$J_x = \frac{1}{2}(J_+ + J_-) .$$

e)

$$J_y = \frac{1}{2i}(J_+ - J_-) .$$

f) $[J_+, J_-] = 2\hbar J_z$.

g)

$$J_{\left\{ \begin{smallmatrix} x \\ y \end{smallmatrix} \right\}}^2 = \pm \frac{1}{4} (J_+^2 + J_-^2 \pm [J_+, J_-]_{\pm}) ,$$

where recall that $[A, B]_{\pm} = AB + BA$ is the anticommutator of A and B .

h)

$$J^2 = \frac{1}{2}[J_+, J_-]_{+} + J_z^2 .$$

013 qfull 00200 2 3 0 mod math: diagonalization of J_x for 3-d

Extra keywords: diagonalization of the J-x angular momentum matrix for 3-d

3. The x -component angular momentum operator matrix in a three-dimensional angular momentum space expressed in terms of the z -component orthonormal basis (i.e., the standard basis with eigenvectors $|1\rangle$, $|0\rangle$, and $|-1\rangle$) is:

$$J_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} .$$

Is this matrix Hermitian? Diagonalize this matrix: i.e., solve for its eigenvalues and normalized eigenvectors (written in terms of the standard basis ket eigenvectors) or, if you prefer in column vector form. Note the solution is somewhat simpler if you solve the reduced eigen problem. Just divide both sides of the eigen equation by $\hbar/\sqrt{2}$ and solve for the reduced eigenvalues. The physical eigenvalues are the reduced ones times $\hbar/\sqrt{2}$.

Verify that the eigenvectors are orthonormal.

NOTE: Albeit some consider it a sloppy notation since kets and bras are abstract vectors and columns vectors are a concrete representation, its concretely useful to equate them at times. In the present case, the kets equate like so

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

and the bras, like so

$$\langle 1| = (1, 0, 0)^*, \quad \langle 0| = (0, 1, 0)^*, \quad \text{and} \quad \langle -1| = (0, 0, 1)^*.$$

013 qfull 00300 2 3 0 mod math: diagonalization. of J_y for 3-d

Extra keywords: diagonalization of the J-y angular momentum matrix for 3-d

4. The y -component angular momentum operator matrix in a three-dimensional angular momentum space expressed in terms of the z -component orthonormal basis (i.e., the standard basis with eigenvectors $|1\rangle$, $|0\rangle$, and $|-1\rangle$) is:

$$J_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

Is this matrix Hermitian? Diagonalize this matrix: i.e., solve for its eigenvalues and normalized eigenvectors (written in terms of the standard basis kets) or, if you prefer in column vector form. Verify that the eigenvectors are orthonormal. Note the solution is somewhat simpler if you solve the reduced eigen problem. Just divide both sides of the eigen equation by $\hbar/\sqrt{2}$ and solve for the reduced eigenvalues. The physical eigenvalues are the reduced ones times $\hbar/\sqrt{2}$.

NOTE: Albeit some consider it a sloppy notation since kets and bras are abstract vectors and columns vectors are a concrete representation, its concretely useful to equate them at times. In the present case, the kets equate like so

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

and the bras, like so

$$\langle 1| = (1, 0, 0)^*, \quad \langle 0| = (0, 1, 0)^*, \quad \text{and} \quad \langle -1| = (0, 0, 1)^*.$$

013 qfull 00400 2 3 0 mod math: angular momentum eqn. of motion

Extra keywords: (Gr-150:4.21) torque

5. Let's consider the angular momentum equation of motion in the context of quantum mechanics.

a) Prove that

$$\frac{d\langle \vec{L} \rangle}{dt} = \langle \vec{\tau} \rangle,$$

where $\vec{L} = \vec{r} \times \vec{p}$ is the angular momentum operator and $\vec{\tau} = \vec{r} \times (-\nabla V)$ is the torque operator.

b) Then prove that

$$\frac{d\langle \vec{L} \rangle}{dt} = 0$$

for any central potential system: i.e., a system where the potential depends on radius alone.

HINTS: You'll need to use the general time evolution equation—or equation of motion or derivative of expectation value: whatever one calls it—people do seem to avoid giving it a name. Then you will need to work out a commutation relation with a cross product operator. There are two approaches. First, show what the commutation relation is component by component. But that's for pedestrians. The second way is to use the Levi-Civita symbol with the Einstein summation rule to prove the all commutation relations simultaneously. Part (a) is most easily done using Cartesian coordinates and part (b) using spherical polar coordinates.

013 qfull 00500 2 3 0 moderate thinking: orbital angular momentum

Extra keywords: expectation values, standard deviations, quantum and classical analogs

6. Consider a spinless particle in an eigenstate $|\ell, m\rangle$ of the L^2 and L_z operators: ℓ is the L^2 quantum number and m the L_z quantum number. The set of $|\ell, m\rangle$ states are a complete orthonormal set for angular coordinates. Recall

$$\begin{aligned} L^2|\ell, m\rangle &= \ell(\ell+1)\hbar^2|\ell, m\rangle, \\ L_z|\ell, m\rangle &= m\hbar|\ell, m\rangle, \\ L_{\pm}|\ell, m\rangle &= \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}|\ell, m\pm 1\rangle, \end{aligned}$$

and

$$L_{\pm} = L_x \pm iL_y.$$

- a) Solve for expectation values $\langle L_x \rangle$, and $\langle L_y \rangle$, and standard deviations ΔL_x and ΔL_y .

HINTS: You will need expressions for L_x and L_y in terms of the given operators. Also the everything can be done by operator algebra: there is no need to bring in the spherical harmonics or particular representations of the operators.

- b) Let us now see if there are classical analogs to the results in part (a). Let classical

$$\begin{aligned} L_z &= m\hbar, \\ L_x &= \hbar\sqrt{\ell(\ell+1) - m^2}\cos(\phi) \end{aligned}$$

and

$$L_y = \hbar\sqrt{\ell(\ell+1) - m^2}\sin(\phi),$$

where ϕ is the azimuthal angle of the angular momentum vector. Note $L_x^2 + L_y^2 + L_z^2 = \ell(\ell+1)\hbar^2$. Now solve for the classical $\langle L_x \rangle$ and $\langle L_y \rangle$, and the classical ΔL_x and ΔL_y assuming (i) that ϕ is random in the range $[0, 2\pi]$ and (ii) that $\phi = \omega t$ where ω is a constant angular frequency.

Chapt. 14 Spin

Multiple-Choice Problems

014 qmult 00100 1 4 1 easy deducto-memory: Goudsmit and Uhlenbeck, spin

1. “Let’s play *Jeopardy!* For \$100, the answer is: Goudsmit and Uhlenbeck.
 - a) Who are the original proposers of electron spin in 1925, Alex?
 - b) Who performed the Stern-Gerlach experiment, Alex?
 - c) Who are Wolfgang Pauli’s evil triplet brothers, Alex?
 - d) What are two delightful Dutch cheeses, Alex?
 - e) What were Rosencrantz and Guildenstern’s first names, Alex?

014 qmult 00200 1 1 5 easy memory: eigenvalues of spin 1/2 particle

2. The eigenvalues of a component of the spin of a spin 1/2 particle are always:
 - a) $\pm \hbar$.
 - b) $\pm \hbar/3$.
 - c) $\pm \hbar/4$.
 - d) $\pm \hbar/5$.
 - e) $\pm \hbar/2$.

014 qmult 00300 1 4 2 easy deducto-memory: spin and environment

3. Is the spin (not spin component) of an electron dependent on the electron’s environment?
 - a) Always.
 - b) No. Spin is an intrinsic, unchanging property of a particle.
 - c) In atomic systems, no, but when free, yes.
 - d) Both yes and no.
 - e) It depends on a recount in Palm Beach.

Full-Answer Problems

014 qfull 00100 2 3 0 mod math: diagonalization of y Pauli spin matrix

Extra keywords: (CDL-203:2), but it corresponds to only part of that problem

1. The y -component Pauli matrix (just the y -spin matrix sans the $\hbar/2$ factor) expressed in terms of the z -component orthonormal basis (i.e., the standard z -basis with eigenvectors $|+\rangle$ and $|-\rangle$) is:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} .$$

Diagonalize this matrix: i.e., solve for its eigenvalues and **NORMALIZED** eigenvectors written in terms of the standard z -basis eigenvector kets or, if your prefer, in column vector form for the z -basis. One doesn’t have to literally do the basis transformation of the matrix to the diagonal form since, if one has the eigenvalues, one already knows what that form is. In

quantum mechanics, literally doing the diagonalization of the matrix is often not intended by a diagonalization.

014 qfull 00200 2 3 0 mod math: spin 1/2, spin $S_x + S_y$.

Extra keywords: (Ga-241:9), spin 1/2, spin $S_x + S_y$, diagonalization

2. Consider a spin 1/2 system. Find the eigenvectors and eigenvalues for operator $S_x + S_y$. Say the system is in one of the eigen-states for this operator. What are the probabilities that an S_z measurement will give $\hbar/2$?

014 qfull 00210 1 5 0 easy thinking: electron spin in B-field Hamiltonian

Extra keywords: electron spin in magnetic field Hamiltonian

3. What is the Hamiltonian fragment (piece, part) that describes the energy of an electron magnetic moment in a magnetic field. This fragment in a Schrödinger equation can be separated from the rest of the equation and solved as separate eigenvalue problem. Assume the intrinsic angular momentum operator is \vec{S} and the magnetic field points in the z direction. **HINTS:** Think of the classical energy of a magnetic dipole in a magnetic field and use the correspondence principle. This is not a long question. This question needs rethinking. It's probably OK, but I've got to study Baym p. 310–315ff carefully.

014 qfull 00300 2 5 0 moderate thinking: classical Larmor precession

4. Let's tackle the classical Larmor precession.
 - a) What is Newton's 2nd law in rotational form?
 - b) What is the torque on a magnetic dipole moment $\vec{\mu}$ in a magnetic field \vec{B} ? **HINT:** Any first-year text will tell you.
 - c) Say that the magnetic moment of a system is given by $\vec{\mu} = \gamma \vec{L}$, where γ is some constant and \vec{L} is the system's angular momentum. Say also that there is a magnetic field $\vec{B} = (0, 0, B_z)$. Solve for the time evolution of \vec{L} using Newton's 2nd law in rotational form assuming the initial condition $\vec{L}(t=0) = (L_{x,0}, 0, L_{z,0})$ with $L_{x,0} > 0$. **HINT:** You should get coupled differential equations for two components of \vec{L} . There not so hard to solve. For niceness you should define an appropriate ω .

014 qfull 00400 3 5 0 tough thinking: quantum mech. Larmor spin precession

Extra keywords: Larmor spin precession

5. Consider a spin 1/2 particle with magnetic moment $\vec{M} = \gamma \vec{S}$. The spin space is spanned by the orthonormal basis vectors $|+\rangle$ and $|-\rangle$ of the observable S_z with eigenvalues $\pm \hbar/2$: this basis is the standard spin basis. At a time $t = 0$, the state of the system is $|\Psi(t=0)\rangle = |+\rangle$.
 - (a) If the observable S_x is measured at time $t = 0$, what eigenvalues can be found with what probabilities and what is the expectation value?
 - (b) Say that there is a magnetic field with only a nonzero y -component B_y . The system evolves under the influence of this field. Find the Hamiltonian for the system, calculate the time-dependent state $|\Psi(t)\rangle$ expanded in the eigenvectors of the Hamiltonian **AND** then expanded in the eigenvectors of the standard z basis. **HINT:** It would be good idea to define an ω . Also you will have to repeat part of (a) to find the time zero expansion coefficients. Perhaps recalling the classical expression for the potential energy of magnet moment in a magnetic field will help: $U = -\vec{M} \cdot \vec{B}$.
 - (c) At a general time t we could measure observables S_x , S_y , and S_z . What are the eigenvalues we would observe and with what probabilities? What are the expectation values for the three observables? What is the physical interpretation of the state of the system?

Chapt. 15 Time-Independent Approximation Methods

Multiple-Choice Problems

015 qmult 00100 1 1 1 easy memory: time-independent perturbation

1. Time-independent weak-coupling perturbation theory assumes that the stationary states and eigen-energies of a system can be expanded in convergent power series in a perturbation parameter about, respectively:
 - a) the stationary states and eigen-energies of a solvable system.
 - b) the eigen-energies and stationary states of an unsolvable system.
 - c) the origin.
 - d) the center.
 - e) infinity.

001 qmult 00200 1 1 5 easy memory: zeroth order perturbation

2. The zeroth order perturbation of a system is:
 - a) the most strongly perturbed system.
 - b) the mostest strongly perturbed system.
 - c) the deeply disturbed system.
 - d) the negatively perturbed system
 - e) the unperturbed system.

015 qmult 00300 1 1 2 easy memory: 1st order energy correction

3. The expression

$$E_n^{1st} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle$$

is:

- a) the eigen-energy of eigen-state n to 0th order in perturbation $\lambda H^{(1)}$.
 - b) the eigen-energy of eigen-state n to 1st order in perturbation $\lambda H^{(1)}$.
 - c) the energy of eigen-state n to 2nd order in perturbation $\lambda H^{(1)}$.
 - d) the eigen-state n to 1st order in perturbation $\lambda H^{(1)}$.
 - e) the eigen-state n to 2nd order in perturbation $\lambda H^{(1)}$.

015 qmult 00400 1 4 4 easy deducto-memory: 1st order eigen state correction

4. The expression

$$|\psi_n^{1st}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, k \neq n} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle$$

is:

- a) the eigen-energy of eigen-state n to 0th order in perturbation $\lambda H^{(1)}$.
 - b) the eigen-energy of eigen-state n to 1st order in perturbation $\lambda H^{(1)}$.
 - c) the energy of eigen-state n to 2nd order in perturbation $\lambda H^{(1)}$.
 - d) the eigen-state n to 1st order in perturbation $\lambda H^{(1)}$.
 - e) the eigen-state n to 2nd order in perturbation $\lambda H^{(1)}$.

 015 qmult 00500 1 1 3 easy memory: 2nd order energy correction

5. The expression

$$E_n^{2\text{nd}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle + \lambda^2 \sum_{\text{all } k, k \neq n} \frac{\left| \langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle \right|^2}{E_n^{(0)} - E_k^{(0)}}$$

is:

- a) the eigen-energy of eigen-state n to 0th order in perturbation $\lambda H^{(1)}$.
- b) the eigen-energy of eigen-state n to 1st order in perturbation $\lambda H^{(1)}$.
- c) the energy of eigen-state n to 2nd order in perturbation $\lambda H^{(1)}$.
- d) the eigen-state n to 1st order in perturbation $\lambda H^{(1)}$.
- e) the eigen-state n to 2nd order in perturbation $\lambda H^{(1)}$.

 015 qmult 00600 1 4 1 easy deducto-memory: degeneracy and perturbation

 6. “Let’s play *Jeopardy!* For \$100, the answer is: A common cause for the obvious failure of time-independent weak-coupling perturbation theory.”

- a) What is degeneracy, Alex?
- b) What is perversion, Alex?
- c) What is subversion, Alex?
- d) What is lunacy, Alex?
- e) What is regency, Alex?

 015 qmult 00700 1 1 3 easy memory: equivalent postulates

7. If two postulates are said to be equivalent, then

- a) one can be derived from the other, but not the other from the one.
- b) the other can be derived from the one, but not the one from the other.
- c) each one can be derived from the other.
- d) neither can be true.
- e) both must be true.

 015 qmult 00800 1 4 5 easy deducto-memory: variational principle

 8. “Let’s play *Jeopardy!* For \$100, the answer is: Usually the demand that an action (or action integral) be stationary with respect to arbitrary variation in a function appearing somehow in the integrand.”

- a) What is a Hermitian conjugate, Alex?
- b) What is an unperturbation principle, Alex?
- c) What is a perturbation principle, Alex?
- d) What is an invariation principle, Alex?
- e) What is a variational principle, Alex?

 015 qmult 00900 1 1 3 easy memory: quantum mechanics action

9. In non-relativistic quantum mechanics the action of the usual variation principle is:

- a) the integral of angular momentum.
 - b) the derivative of angular momentum.
 - c) the expectation value of the Hamiltonian.
 - d) the time independent Schrödinger equation.
 - e) the Dirac equation.
-

015 qmult 01000 1 1 1 easy memory: stationary action

10. An exact solution $|\phi\rangle$ to the time-independent Schrödinger equation is the one that by the variational principle in quantum mechanics makes the action

$$E(\phi) = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

be stationary with respect to:

- a) arbitrary variations of the state $|\phi\rangle$ (i.e., $\delta E(\phi) = 0$).
- b) some variations of the state $|\phi\rangle$.
- c) no variations of the state $|\phi\rangle$.
- d) reasonable variations of the state $|\phi\rangle$.
- e) unreasonable variations of the state $|\phi\rangle$.

015 qmult 01100 1 1 5 easy memory: simple variational method

11. In the simple variational method one takes a parameterized wave function and finds the parameters that make the expectation value of the Hamiltonian:
- a) a maximum.
 - b) 1.
 - c) negative.
 - d) positive.
 - e) a minimum.

015 qmult 01200 1 4 3 easy deducto-memory: linear variation method

12. “Let’s play *Jeopardy!* For \$100, the answer is: The justification for the linear variational method (or Rayleigh-Ritz method or truncated Hamiltonian matrix eigen-problem).”
- a) What is Hermitian conjugation, Alex?
 - b) What is bra/ket notation, Alex?
 - c) What is the quantum mechanics variational principle, Alex?
 - d) What is the Dirac principle, Alex?
 - e) What is the cosmological principle, Alex?

015 qmult 01500 1 4 1 easy deducto-memory: repulsion energy levels

13. Any perturbation applied to a two-level system that is initially degenerate causes:
- a) a repulsion of the energy levels.
 - b) an attraction of the energy levels.
 - c) a warm and affectionate relationship between the energy levels.
 - d) a wonderful, meaningful togetherness of the energy levels.
 - e) an eternal soul-bliss of the energy levels.

Full-Answer Problems

015 qfull 00100 2 5 0 moderate thinking: what is a perturbation?

1. What is a perturbation?

015 qfull 00200 2 5 0 moderate thinking: basic perturbation hypothesis

2. What is the basic non-degenerate perturbation method hypothesis?

015 qfull 00300 2 5 0 moderate thinking: smallness parameter

3. What is role of the smallness parameter in non-degenerate perturbation theory?

015 qfull 00400 2 5 0 moderate thinking: 2nd bigger than 1st

4. If all the 2nd order non-degenerate perturbation corrections are greater than the 1st order ones, what might you suspect?

015 qfull 00500 2 5 0 moderate thinking: 2nd bigger than 1st all zero

5. If all the 2nd order non-degenerate perturbation corrections are greater than the 1st order ones, but the 1st order ones were all identically zero, what might you suspect?

015 qfull 00600 1 5 0 easy thinking: equivalent results

6. If two different looking theorems or postulates were said to be equivalent what would that mean?

015 qfull 00700 2 5 0 moderate thinking: variational principle and method

7. Are the variational principle and the variational method the same thing? Explain please.

015 qfull 00800 1 5 0 easy thinking: what is a stationary point?

8. What does it mean to say a function is stationary at a point?

015 qfull 00800 2 3 0 moderate math: differentiation

9. Take the derivative of

$$E(\alpha) = \frac{5}{4} \frac{\hbar^2}{m\alpha^2} + \frac{1}{14} m\omega^2 \alpha^2$$

and determine the stationary point. Just by imagining the function's behavior in the large and small α limits determine whether the stationary point is a minimum. Give the analytic expression for $E(\alpha)$ at the stationary point.

015 qfull 00900 2 5 0 moderate thinking: Snell's law and var. princ.

10. Can Snell's law be derived using the variational principle (or a variational principle "as you prefer")? Please explain.

015 qfull 01000 2 5 0 moderate thinking: Schröd. and var. princ.

11. Can the time-independent Schrödinger's equation be derived using the variational principle? Please explain.

015 qfull 01100 2 5 0 moderate thinking: expand in basis

12. Convert the bracket eigenproblem $H|\Psi\rangle = E|\Psi\rangle$ to the discrete $\{|u_j\rangle\}$ orthonormal basis representation by expanding $|\Psi\rangle$ in terms of the $|u_j\rangle$ kets and then operating on the equation with the bra $\langle u_i|$.

015 qfull 01200 1 5 0 easy thinking: solving infinite matrix problem

13. Can one literally solve in a numerical procedure an infinite matrix problem: i.e. a problem with an infinite number of terms to number crunch? Why so or why not?

015 qfull 01300 1 5 0 easy thinking: diagonalization defined

14. What is meant by diagonalization in quantum mechanics?

015 qfull 01400 2 3 0 moderate math: Dirac delta perturbation

Extra keywords: (Gr-225:6.1) Dirac delta perturbation, 1-dimensional infinite square well

15. Say you have a one-dimensional square well with

$$V(x) = \begin{cases} 0, & \text{for the } x \text{ range } 0 \text{ to } a; \\ \infty, & \text{otherwise.} \end{cases}$$

- a) Solve for the stationary states from the Schrödinger equation.
- b) Say we add Dirac delta function perturbation

$$H^{(1)} = c\delta(x - a/2) .$$

What is the general expression for this perturbation for the first order perturbation energy correction?

015 qfull 01410 3 5 0 tough thinking: 2-particle Dirac delta perturbation

Extra keywords: (Gr-226:6.3)

16. The single particle stationary states and eigen-energies for a 1-dimensional infinite square well for region $[0, a]$ are, respectively,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad \text{and} \quad E_n = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 n^2 .$$

- a) What is the expression for elementary 2-particle stationary states for **NON**-identical particles of the same mass? (Label the particles a and b for convenience and assume the particles are spinless. Label the states n and n' for convenience too.) What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies (i.e., $n^2 + n'^2$) up $n = n' = 7$? These energies can be called energy levels: the levels may correspond to more than one state. (You are permitted to use a computer program to generate these.) Are there any degeneracies with these energies? Remember the particles are not identical.
- b) Now suppose we turn on a perturbation potential for the non-identical particles of the form

$$H^{(1)} = V(x_a, x_b) = aV_0\delta(x_a - x_b) .$$

What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_a, x_b) | H^{(1)} | \psi_{nn'}(x_a, x_b) \rangle .$$

If you expand $\sin \theta$ in exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n \neq n'$ and $n = n'$ a bit differently. Given the diagonal matrix elements can you do (weak-coupling) perturbation theory on all the 2-particle states?

- c) What is the expression for elementary 2-particle stationary states for identical spinless bosons? (Label the particles a and b for convenience. Note we have turned off the perturbation.) What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies (i.e., $n^2 + n'^2$) up $n = n' = 7$? (You don't have to do part (a) all over again, just mutatis mutandis it.) Are there any degeneracies with these energies? Remember the particles are identical.
- d) Now suppose we turn on a perturbation potential of part (b) for the identical bosons. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_a, x_b) | H^{(1)} | \psi_{nn'}(x_a, x_b) \rangle .$$

If you expand $\sin \theta$ in exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n \neq n'$ and $n = n'$ a bit differently. Note the perturbation correction is a bit different from the non-identical particle case. Why? Given the matrix elements can you do (weak-coupling) perturbation theory on all the 2-particle states?

- e) What is the expression for elementary 2-particle stationary states for identical fermions when we assume spin coordinates are identical. Since the spin coordinates are identical,

the spin part of the single particle states are symmetrical. Don't bother writing down spinors or such. (Label the particles a and b for convenience. Note we have turned off the perturbation.) What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies (i.e., $n^2 + n'^2$) up $n = n' = 7$? (You don't have to do part (a) all over again, just mutatis mutandis it.) Are there any degeneracies with these energies? Remember the particles are identical.

- f) Now suppose we turn on a perturbation potential of part (b) for the identical fermions. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_a, x_b) | H^{(1)} | \psi_{nn'}(x_a, x_b) \rangle .$$

Don't whine: this is easy if you see the trick. Why do you get the simple result you get? Given the matrix element, can you do (weak-coupling) perturbation theory on all the 2-particle states?

- g) What does the Dirac delta potential

$$V(x_a - x_b) = aV_0(x_a - x_b)$$

imply or do physically?

015 qfull 01500 1 3 0 easy math: SHO 1st order perturbation cx

Extra keywords: SHO 1st order perturbation cx

17. Say you add a perturbation potential cx to a 1-dimensional simple harmonic oscillator (SHO) system. Calculate all the first order weak-coupling perturbation corrections for the eigen-energies. Recall the 1st order perturbation energy correction is given by

$$E_n^{(1)} = \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle = 0 ,$$

where the $|\psi_n^{(0)}\rangle$ are unperturbed eigenstates. **HINT:** Think about the parity of SHO energy eigenstates.

015 qfull 01600 2 3 0 mod math: SHO exact cx perturbation

Extra keywords: (Gr-227:6.5), SHO, linear perturbation cx , exact cx solution

18. Say you added a perturbation $H^{(1)} = cx$ to the 1-dimensional simple harmonic oscillator (SHO) Hamiltonian, and so have

$$H = \frac{p^2}{2m} + \frac{1}{2}mw^2x^2 + cx$$

for the Hamiltonian. An exact solution to the time independent Schrödinger equation is in fact possible and easy since the new problem is still a SHO problem.

- a) Let's consider just the mathematical aspects of the problem first. Given a quadratic

$$y = ax^2$$

with $a > 0$, where is its minimum and roots? Say you now add bx to get

$$y = ax^2 + bx .$$

Where are the minimum and roots now? By measuring the horizontal coordinate from a new origin is it possible to eliminate the linear dependence on the horizontal coordinate? Find this new origin. From a geometric point of view what have you done by adding bx to $y = ax^2$: i.e., what has happened to the parabola on the plane?

- b) Now that the math is clear what about the physics. What are the classical forces associated with the potentials

$$\frac{1}{2}m\omega^2 x^2, \quad cx, \quad \text{and} \quad \frac{1}{2}m\omega^2 x^2 + cx ?$$

What are the equilibrium points of the forces? What are the potential energies of the first and third equilibrium points? What has adding the cx potential done to the potential well of the SHO? How could you reduce the problem with the third potential to that with the first?

- c) Now reduce time independent Schrödinger problem with the given Hamiltonian to the SHO problem. What are the solutions in terms of horizontal coordinate distance from the new origin and what are eigen-energies of the solutions? (I don't mean solve for the solutions. Just what are known solutions for reduced problem.)

015 qfull 01700 3 3 0 mod math: SHO and 2nd order perturbation cx

Extra keywords: SHO and 2nd order perturbation cx

19. Say you add a perturbation potential cx to a 1-dimensional simple harmonic oscillator (SHO) system. Give the formula for the 2nd order weak coupling perturbation correction for this special case simplified as much as possible. **HINT:** You will probably find the following matrix element formula for SHO eigenvectors useful:

$$\langle \Psi_k | x | \Psi_n \rangle = \begin{cases} \frac{1}{\beta} \sqrt{\frac{\max(k, n)}{2}} & \text{if } |k - n| = 1; \\ 0 & \text{otherwise,} \end{cases}$$

where $\beta = \sqrt{m\omega/\hbar}$ (e.g., Mo-406).

015 qfull 03000 3 3 0 tough math: SHO and 2nd order x^3 pre-perturbation

Extra keywords: SHO and 2nd order x^3 pre-perturbation

20. In preparation for calculating the 1st order perturbation wave function correction and the 2nd order perturbation energy correction for the 1-dimensional simple harmonic oscillator (SHO) system with perturbation potential cx^3 , one needs to find a general expression for

$$\langle \psi_k | x^3 | \psi_n \rangle .$$

Find this expression simplified as much as possible.

INSTRUCTIONS: You will need the following to formulae (which I hope are correct)

$$\frac{1}{\sqrt{2}\beta} [\sqrt{n+1}\psi_{n+1}(x) + \sqrt{n}\psi_{n-1}(x)] = x\psi_n(x)$$

and

$$\langle \psi_k | x^2 | \psi_n \rangle = \begin{cases} \frac{2n+1}{2\beta^2} & \text{if } k = n; \\ \frac{\sqrt{[\max(k, n) - 1] \max(k, n)}}{2\beta^2} & \text{if } |k - n| = 2; \\ 0 & \text{otherwise,} \end{cases}$$

where $\beta = \sqrt{m\omega/\hbar}$. There are seven initial cases (one being zero) to find and five final cases after combining initial cases with same k and n relation. Write the expressions in terms of n , not k . You will simply have to work carefully and systematically to grind out the cases. What is the appropriate Kronecker delta function to go with each case so that one can put them

in a sum over k in the 2nd order perturbation formulae? Make the Kronecker deltas in the form $\delta_{k,f(n)}$ where $f(n)$ is an expression like, e.g., $n-1$. Since k in the sum for the 2nd order perturbation runs only from zero to infinity is there any special treatment needed for including cases with Kronecker deltas like $\delta_{k,n-1}$ for $n=0$? **HINT:** Are such cases ever non-zero when they should be omitted?

015 qfull 03100 3 3 0 mod math: SHO and 2nd order cx^3 perturbation

Extra keywords: SHO and 2nd order cx^3 perturbation

21. The following result is for simple harmonic oscillator eigenvectors:

$$\langle \psi_k | x^3 | \psi_n \rangle = \frac{1}{2\sqrt{2}\beta^3} \begin{cases} 3(n+1)\sqrt{n+1} & \text{if } k = n+1 \text{ with } \delta_{k,n+1}; \\ 3n\sqrt{n} & \text{if } k = n-1 \text{ with } \delta_{k,n-1}; \\ \sqrt{(n+1)(n+2)(n+3)} & \text{if } k = n+3 \text{ with } \delta_{k,n+3}; \\ \sqrt{(n-2)(n-1)n} & \text{if } k = n-3 \text{ with } \delta_{k,n-3}; \\ 0 & \text{otherwise.} \end{cases}$$

Using this expression find the general expression for the SHO for the 2nd order weak-coupling perturbation corrections to the eigenstate energies for a perturbation potential cx^3 . Why can you use the expression above without worrying about the fact that sum over states from zero to infinity doesn't include states with index less than zero.

015 qfull 03110 2 5 0 moderate thinking: 4x4 eigenproblem/perturbation

22. You are given a zeroth order Hamiltonian matrix

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

- a) Solve for the eigenvalues and normalized eigenvectors by inspection. You should label the states 1, 2, 3, and 4 for convenience. Is there any degeneracy and if so what the degenerate states?
- b) The evil wizard of physics now turns on a perturbation and the Hamiltonian becomes

$$H = \begin{pmatrix} 1 & \epsilon & 0 & 0 \\ \epsilon & 1 & 0 & 0 \\ 0 & 0 & 1 & \epsilon \\ 0 & 0 & \epsilon & -1 \end{pmatrix},$$

where ϵ is a small quantity. Solve for the exact eigenvalues and normalized eigenvectors in this case. Is there any degeneracy now? **HINT:** Is there any reason why the two 2×2 blocks in the matrix cannot be treated as separate eigenvalue problems and the two-component eigenvectors extended trivially for the 4×4 problem?

- c) Do weak-coupling perturbation theory to solve for the energy to 2nd order for any initial eigenstates which are not degenerate. **HINT:** All the perturbation matrix elements can be found in the part (b) question.

015 qfull 03200 2 5 0 moderate thinking: simple variational method, excited states

23. The simple variational method can in principle be applied to excited states.

- a) Say an unnormalized trial wave function $|\psi\rangle$ is orthogonal to all energy eigenstates $|\phi_i\rangle$ of quantum number less than n , where the eigen-energies increase monotonically with

quantum number as usual. Show that $E_{\text{trial}} \geq E_n$ where E_{trial} is the expectation value of the Hamiltonian for $|\psi\rangle$. When will the equality hold? Remember there is such a thing as degeneracy.

- b) Using the simple variational method for finding excited eigenstate energies isn't really of general interest since constructing trial functions with the right orthogonality properties is often harder than using the other approaches. However, if the eigenstates have definite parity, definite parity trial wave functions can be used to determine the lowest eigen-energies for wave functions of each kind of parity.

For example, let us consider the simple harmonic oscillator problem in one dimension. We know that the eigenstates are non-degenerate and have definite parity. It is given that the ground state has even parity and the first excited state has odd parity. We can use an odd trial wave function and the variational method to approximately determine the energy of the first excited state. The simple harmonic oscillator eigenproblem in scaled dimensionless variables is

$$\left(-\frac{d^2}{dx^2} + x^2\right)\psi = E\psi ,$$

where

$$x = \sqrt{\frac{m\omega}{\hbar}} x_{\text{phy}} \quad \text{and} \quad E = \frac{E_{\text{phy}}}{\hbar\omega/2} = 2n + 1 .$$

The n is the SHO energy quantum number (n runs $0, 1, 2, 3, \dots$) and the “phy” stands for physical. Consider the odd trial wave function

$$\psi = \begin{cases} x(x^2 - c^2), & |x| \leq c; \\ 0, & |x| > c, \end{cases}$$

where c is a variational parameter. Normalize this trial wave function, evaluate its expectation energy, and minimize the expectation energy by varying c . How does this variational method energy compare to the exact result which in scaled variables is 3.

HINT: There are no wonderful tricks in the integrations: grind them out carefully.

015 qfull 03300 3 5 0 tough thinking: perturbation and variation

Extra keywords: (Gr-235:6.9)

24. Consider quantum system of 3 dimensions with initial Hamiltonian

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

and perturbed Hamiltonian

$$H = \begin{pmatrix} 1 - \epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} .$$

Note we assume $\epsilon \ll 1$. Also note that $H^{(0)}$ and H are matrix Hamiltonians: i.e., Hamiltonians in a particular representation. The matrix elements are $\langle \phi_i | H_{\text{op}}^{(0)} | \phi_k \rangle$, $\langle \phi_i | H_{\text{op}} | \phi_k \rangle$, respectively, where $H_{\text{op}}^{(0)}$ and H_{op} are operator versions of the Hamiltonian and $\{|\phi_i\rangle\}$ are some orthonormal basis. Usually we drop the “op” subscript and allow context to tell whether the Hamiltonian is in matrix or operator representation.

- a) Solve by inspection for the eigen-energies and eigenvectors of the initial unperturbed Hamiltonian. To help with the rest of the problem label the states 1, 2, and 3 in some sensible order.

- b) Solve for the exact eigen-energies and normalized eigenvectors of the perturbed Hamiltonian. No need to be too explicit about the eigenvectors. **HINTS:** It's not so hard—if you don't make a mistake in the first step.
- c) Expand the exact eigen-energies and eigenvectors (where applicable) to 2nd order in small ϵ . (Note I mean Taylor expansion, not perturbation series expansion although the two expansion are closely related in this case.) Simplify the eigenvectors to nice forms so that it is easy to see which perturbed vector grew out of which unperturbed vector as ϵ grew from 0.
- d) Determine from (weak-coupling) perturbation theory the energies to 2nd order and the eigenvectors to 1st order of the perturbed Hamiltonian. How do these results compare with those of the part (c) answer? **HINT:** Perturbation theory can be applied to the degenerate states in this case because they are completely uncoupled.
- e) Now use the truncated Hamiltonian matrix method (or linear variational method) to find approximate eigen-energies and eigenvectors for the two initially degenerate eigen-energy states. To what order goodness in small ϵ are the results? Why the are results for one perturbed state exact and for the other rather poor compared to the exact results?

015 qfull 04000 3 5 0 tough thinking: variational hydrogen

Extra keywords: (Ha-327:4.1)

25. We know, of course, the ground state for the hydrogenic atom sans perturbations:

$$\psi_{n\ell m} = \frac{1}{\sqrt{4\pi}} (2a^{-3/2}) e^{-r/a} ,$$

where $a = a_0/[(m/m_e)Z]$ is the radial scale parameter: $a_0 = \hbar^2/(m_e e^2) = \lambda_{\text{Compton}}/(2\pi\alpha) = 0.529 \text{ \AA}$ is the Bohr radius, m is the reduced mass, and Z is the nuclear charge (Gr-128, 141). But as a tedious illustration of the simple variational method, let us try find an approximate ground state wave function and energy starting with the trial Gaussian wave function

$$\psi = A e^{-\beta r^2/a^2} .$$

- a) Can we obtain the exact solution with a trial wave function of this form?
- b) The varied energy is given by

$$E_v = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_0^\infty [\psi(r)^* H \psi(r)] (4\pi r^2) dr}{\int_0^\infty [\psi(r)^* \psi(r)] (4\pi r^2) dr} ,$$

where H is the Hamiltonian for $\ell = 0$ (i.e., the zero angular momentum case) given by

$$H = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{Ze^2}{r} .$$

Note the varied energy form does not require a Lagrange undetermined multiplier since we are building the constraint of normalization into the variation. We, of course, need to evaluate A later to normalize the minimized wave function. Convert the varied energy expression into a dimensionless form in terms of the coordinate $x = r/a$ and reduced varied energy $\epsilon_v = E_v/[Ze^2/(2a)] = Z^{-2}(m/m_e)E_v/E_{\text{Ryd}} \approx Z^{-2}(m/m_e)E_v/(13.606 \text{ eV})$. **HINT:** A further integration transformation can make the analytic form even simpler.

- c) Find the explicit analytic expression for ϵ_v . Sketch a plot of ϵ_v as a function of β . **HINT:** Use an integral table.
- d) Now find the minimizing β value and the minimum ϵ_v . Compare ϵ_v to exact ground state value which is -1 in fact.

Chapt. 16 Time-Dependent Perturbation Theory

Multiple-Choice Problems

016 qmult 00100 1 1 4 easy memory: Fermi, person identification

Extra keywords: Fermi, person identification

1. Who was Enrico Fermi?
 - a) An Italian who discovered America in 1492.
 - b) An Italian who did not discover America in 1492.
 - c) An Italian-American biologist.
 - d) An Italian-American physicist.
 - e) Author of *Atoms in the Family*.

016 qmult 00200 1 1 5 easy memory: electric dipole selection rules

Extra keywords: electric dipole selection rules

2. The selection rules for electric dipole transitions are:
 - a) $\Delta l = 0$ and $\Delta m = 0$.
 - b) $\Delta l = \pm 2$ and $\Delta m = \pm 1$.
 - c) $\Delta l = -1$ and $\Delta m = 1$.
 - d) $\Delta l = \pm 1$ and $\Delta m = 0$.
 - e) $\Delta l = \pm 1$ and $\Delta m = 0, \pm 1$.

016 qmult 00300 1 1 5 easy memory: harmonic perturbation, sinusoidal

Extra keywords: harmonic perturbation, sinusoidal time dependence

3. Harmonic perturbations have:
 - a) a linear time dependence.
 - b) a quadratic time dependence.
 - c) an inverse time dependence.
 - d) an exponential time dependence.
 - e) a sinusoidal time dependence.

Full-Answer Problems

016 qfull 00100 1 5 0 easy thinking: time-dependent Sch.eqn.

1. Is the time-dependent Schrödinger equation needed for time-dependent perturbation theory?

016 qfull 00200 2 5 0 moderate thinking: energy eigenstates

2. Are stationary states (i.e., energy eigenstates) needed in time-dependent perturbation theory? Please explain.

016 qfull 00300 2 5 0 moderate thinking: energy eigenstates

3. What is done with the radiation field in quantum electrodynamics.

016 qfull 00100 2 3 0 easy math: Fermi's golden rule integral

Extra keywords: Fermi's golden rule integral, Simpson's rule

4. By some means evaluate

$$\int_{-\pi}^{\pi} \frac{\sin^2 x}{x^2} dx .$$

The integral is not analytically solvable. One could use a numerical technique like Simpson's rule. On the other hand one could simply find a function that is integrable that sort of resembles the integrand and use that as an approximation. This integral comes up in understanding Fermi's golden rule for time-dependent perturbation.

014 qfull 00200 3 3 0 tough math: time dependent perturbation, square well

Extra keywords: (MEL-141:5.3), time dependent perturbation, infinite square well

5. At time $t = 0$, an electron is in the $n = 1$ eigenstate of an infinite square well with potential

$$V(x) = \begin{cases} 0, & x \in [0, a]; \\ \infty & x > a. \end{cases}$$

At that time an electric field E pointed in the positive x direction is suddenly applied. Use 1st order time-dependent perturbation theory to calculate the transition probabilities to all other states as a function of time. **HINT:** The sinusoidal eigenfunctions can be expressed as exponentials: let $z = \pi x/a$, and then

$$\sin(nz) = \frac{e^{inz} - e^{-inz}}{2i} .$$

014 qfull 00300 3 5 0 tough thinking: usual and general Fermi's golden rule

6. Say we have time-dependent perturbation

$$H(t) = \begin{cases} 0, & t < 0; \\ H, & t \geq 0, \end{cases}$$

and initial state $|\phi_j\rangle$, where $|\phi_j\rangle$ is eigenstate belonging to the complete set $\{|\phi_i\rangle\}$. The state at any time $t \geq 0$ is $|\Psi(t)\rangle$.

- Work out as far as one reasonably can the 1st order perturbation expression for the coefficient $a_i(t)$ in the expansion of $|\Psi(t)\rangle$ in terms of the set $\{|\phi_i\rangle\}$. Include the case of $i = j$. **HINT:** The worked out expression should contain a sine function. Define $\omega_{ij} = (E_i - E_j)/\hbar$.
- Given $i \neq j$, find the transition probability (to 1st order of course) from state j to state i .
- What is this probability at early times when $\omega_{ij}t/2 \ll 1$ for all possible ω_{ij} ? Describe the behavior of the probability as a function of time for all times. (You could sketch a plot of probability as a function of time.) What is the behavior for $\omega_{ij} = 0$ (i.e., for transitions to degenerate states)?
- Assume there is a high enough density of states that the total transition probability to states $i \neq j$ in sum energy interval E_a to E_b can be approximated by an integral:

$$P(t) = \sum_{i \neq j} P_i(t) \approx \int_{E_a}^{E_b} P(E, t) \rho(E) dE ,$$

where $\rho(E)$ is the density of states per unit energy and where the time-independent part of the matrix element H_{ij} is replaced by $H(E)$ which is a continuous function of energy. What is the total transition probability to all states assuming that $|H(E)|^2$ and $\rho(E)$ are constant and so can be removed from the integral and assuming the lower limit of the integral can be set to negative infinity with negligible error? (Note you will probably need to look up a standard definite integral.)

In fact 90 % of the integral (assuming $|H(E)|^2$ and $\rho(E)$ constant) comes from the energy range $[E_j - 2\pi\hbar/t, E_j + 2\pi\hbar/t]$. (Can you show this by a numerical integration? No extra credit for doing this: insight is the only reward.) We can see that at some time the 90 %-range will be so narrow that the approximation $|H(E)|^2$ and $\rho(E)$ constant will probably become valid. They should clearly be evaluated at E_j . Practically, this often means that the approximation becomes valid when almost all of the transitions are to nearly degenerate states. Of course, the 90 %-range can become so narrow that the approximation of a continuum of states breaks down and then the integration becomes invalid again.

What is the rate of transition for (i.e., time derivative of) this total transition probability? The transition rate result is one of the usual forms of Fermi's golden rule. Although it is restricted in many ways, it is still a very usual result: hence golden.

- e) Let's see if we can derive a Fermi's golden rule without the restriction that the perturbation is constant after a sudden turn-on. To do this assume that

$$H(t) = H f(t) ,$$

where H is now constant with time and $f(t)$ is a real turn-on function with the properties that $f(t) = 0$ for $t \leq t_0$ and $f(t) = 1$ for $t \geq t_1$. Again derive $P_i(t)$ leaving it in double integral form. Then, assuming the exponential in the integrand is sharply peak near E_j , solve for the total transition probability an integration over energy using $\rho(E)$ for the energy density of states again. You will need the result

$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{-ikx}}{2\pi} dk ,$$

where $\delta(x)$ is the Dirac delta function. What is the total transition probability when $t \geq t_1$? What is the total transition rate when $t \geq t_1$? How does this new Fermi's golden rule compare to the one in part (d)?

Chapt. 17 The Hydrogenic Atom and Spin

Multiple-Choice Problems

017 qmult 00100 1 1 4 easy memory: spin-orbit interaction, hydrogenic atom

Extra keywords: spin-orbit interaction, hydrogenic atom

1. What is the main perturbation preventing the spinless hydrogenic eigenstates from being the actual ones?
 - a) The Stark effect.
 - b) The Zeeman effect.
 - c) The Stern-Gerlach effect.
 - d) The spin-orbit interaction.
 - e) The Goldhaber interaction.

017 qmult 00200 2 4 5 moderate deducto-memory: orbital ang. mom., spin

Extra keywords: orbital angular momentum, spin, total angular momentum

2. The scalar product of operators $\vec{L} \cdot \vec{S}$ equals
 - a) J^2 .
 - b) $(\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S})$.
 - c) $(\vec{L} - \vec{S}) \cdot (\vec{L} - \vec{S})$.
 - d) $(J^2 + L^2 + S^2)/2$.
 - e) $(J^2 - L^2 - S^2)/2$.

017 qmult 00300 1 4 3 easy deducto-memory: spin-orbit good quantum numbers

Extra keywords: spin-orbit interaction, good quantum numbers

3. “Let’s play *Jeopardy!* For \$100, the answer is: The spin-orbit interaction causes the eigenstates of the real hydrogen atom to be mixtures of the $\Psi_{n\ell m}$ states, but one $\Psi_{n\ell m}$ state is usually overwhelmingly dominant.
 - a) Why are the quantum numbers n , ℓ , and m perfectly rotten, Alex?
 - b) Why are the quantum numbers n , ℓ , and m only approximately rotten, Alex?
 - c) Why are the quantum numbers n , ℓ , and m only approximately good, Alex?
 - d) Why are the quantum numbers n , ℓ , and m only indifferent, Alex?
 - d) Why are the quantum numbers n , ℓ , and m dependent on a recount in Palm Beach, Alex?

Full-Answer Problems

Chapt. 18 Multi-Particle System

Multiple-Choice Problems

018 qmult 01000 1 4 5 easy deducto-memory: Bose-Einstein condensate

Extra keywords: References Gr-216, CDL-1399, Pa-179

1. “Let’s play *Jeopardy!* For \$100, the answer is: The name for the state of a system of all identical bosons when the bosons all settle into the ground state.”
 - a) What is a Hermitian conjugate, Alex?
 - b) What is a Hermitian condensate, Alex?
 - c) What is a Rabi-Schwinger-Baym-Sutherland-Jeffery degeneracy, Alex?
 - d) What is just another state, Alex?
 - e) What is a Bose-Einstein condensate, Alex?

Full-Answer Problems

018 qfull 02000 2 5 0 moderate thinking: symmetrization

Extra keywords: symmetrization of orthonormal single particle states.

1. Say $|ai\rangle$ and $|bi\rangle$ are **ORTHONORMAL** single particle states, where i is a particle label. The label can be thought of as labeling the coordinates to be integrated or summed over in an inner product: see below. The symbolic combination of such states for two particles, one in a and one in b is

$$|12\rangle = |a1\rangle|b2\rangle ,$$

where 1 and 2 are particle labels. This combination is actually a tensor product, but let’s not worry about that now. The inner product of such a combined state is written

$$\langle 12|12\rangle = \langle a1|a1\rangle\langle b2|b2\rangle .$$

If one expanded the inner product in the position and spinor representation assuming the wave function and spinor parts can be separated (which in general is not the case),

$$\begin{aligned} \langle 12|12\rangle &= \left[\int \psi_a(x_1)^* \psi_a(x_1) dx_1 \begin{pmatrix} c_{1+}^* & c_{1-}^* \end{pmatrix}_a \begin{pmatrix} c_{1+} \\ c_{1-} \end{pmatrix}_a \right] \\ &\times \left[\int \psi_b(x_2)^* \psi_b(x_2) dx_2 \begin{pmatrix} c_{2+}^* & c_{2-}^* \end{pmatrix}_b \begin{pmatrix} c_{2+} \\ c_{2-} \end{pmatrix}_b \right] . \end{aligned}$$

A lot of conventions go into the last expression: don’t worry too much about them.

- a) Let particles 1 and 2 be **NON**-identical particles. What are the two simplest and most obvious normalized 2-particle states that can be constructed from states a and b ? What happens if $a = b$ (i.e., the two single particle states are only one state actually)?
- b) Say particles 1 and 2 are identical bosons or fermions. What is the simplest and most obvious normalized 2-particle state that can be constructed in either case allowing for the possibility

that $a = b$ (i.e., the two single particle states are only one state actually)? What happens if $a = b$, for fermions.

018 qfull 02100 1 5 0 easy thinking: triplet singlet

Extra keywords: (Gr-181:5.3)

2. Say that we have obtained four orthonormal single particle eigenstates:

$$\psi_a(\vec{r})\chi_+$$

$$\psi_a(\vec{r})\chi_-$$

$$\psi_b(\vec{r})\chi_+$$

and

$$\psi_b(\vec{r})\chi_-$$

where the spinors are

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{or} \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

To label a state i's coordinates by a descriptive label one can write for example

$$\psi_a(i)(\vec{r})\chi_+(i) .$$

Construct ????

018 qfull 02200 3 5 0 tough thinking: 2-particle infinite square well

Extra keywords: (Gr-182:5.4)

3. The set of individual eigen states for a 1-dimensional, infinite square well confined to $[0, a]$ can be written $|n\rangle$ where $n = 1, 2, 3, \dots$. The energies of the states are given by

$$E(n) = \frac{\hbar^2}{2m} \left(\frac{\pi}{a} \right)^2 n^2$$

(e.g., Gr-26). For convenience $E_{\text{red}}(n) = n^2$ can be called the reduced energy of state n .

- a) Say we have two non-interacting particles a and b in the well. Write down the Hamiltonian for this case. The particles have the same mass m , but are not necessarily identical.
- b) The reduced energy of a 2-particle state that satisfy the Schrödinger equation of part (a) can be written

$$E_{\text{red}}(n_1, n_2) = n_1^2 + n_2^2 .$$

Write a small computer code to exhaustively calculate the possible reduced energy levels up to and including $E_{\text{red}} = 50$ and the n_1 and n_2 combinations that yield these energies. The code should also calculate the degeneracy of each energy for the cases of non-identical particles, bosons, and fermions. I'll left you off easily, accidental degeneracies can be identified by eye. (Note: An accidental degeneracy is when a distinct pair of n values (i.e., a pair not counting order) gives the same reduced energy.)

- c) Write down the normalized vector expressions for all the 2-particle states up to the 4th allowed energy level for the cases of non-identical particles, identical bosons, and identical fermions. Just to get you started the non-identical particle ground state is

$$|a1, b1\rangle = |a1\rangle|b1\rangle \quad \text{with} \quad E_{\text{red}} = 2 .$$

018 qfull 02300 3 5 0 tough thinking: exchange force

Extra keywords: (Gr-182)

4. The exchange force is a pseudo-force that arise because of the symmetry postulate of quantum mechanics. Say we have orthonormal individual particle states $|a\rangle$ and $|b\rangle$. If we have distinguishable particles 1 and 2 in $|a\rangle$ and $|b\rangle$, respectively, the net state is

$$|1, 2\rangle = |a1\rangle|b2\rangle .$$

Of course, each of particles 1 and 2 could be in linear combinations of the two states. In that case the combined state would be a four term state. But we have no interest in pursuing that digression at the moment. Now 2 indistinguishable particles in states $|a\rangle$ and $|b\rangle$ have no choice, but to be in a combined symmetrized state by the symmetry postulate:

$$|1, 2\rangle = \frac{1}{\sqrt{2}} (|a1\rangle|b2\rangle \pm |b1\rangle|a2\rangle) ,$$

where the upper case is for identical bosons and the lower case for identical fermions. If the two states are actually the same state $|a\rangle$, then the state for distinguishable particles and bosons is the same

$$|1, 2\rangle = |a1\rangle|a2\rangle$$

and no state is possible for fermions by the Pauli exclusion principle.

Note products of kets are actually tensor products (CDL-154). In taking scalar products, the bras with index i (e.g., 1 or 2 above) act on the kets of index i . For example, for the state $|1, 2\rangle = |a1\rangle|a2\rangle$ the norm squared is

$$\langle 1, 2|1, 2\rangle = \langle a1|a1\rangle\langle a2|a2\rangle .$$

The fact that identical particles must be combined symmetrized states means that their wave functions will be more or less clumped depending on whether they are bosons or fermions than if they could be fitted into simple product states like distinguishable particles. (Note we are not bothering with the complication of spin for the moment. One could say we are letting all the spins point up for example). This clumping/declumping effect is called the exchange force. Obviously, it is not really a force, but rather a result of the requirements on allowed states. Still for some practical purposes one can certainly consider it as force.

- Expand $\langle \Delta x^2 \rangle = \langle (x_1 - x_2)^2 \rangle$.
- For the given states, determine $\langle \Delta x^2 \rangle$ for distinguishable particles and, for the case of being only one single particle state $|a\rangle$, for indistinguishable bosons.
- For the given states constructed from distinct single particle states, determine $\langle \Delta x^2 \rangle$ for indistinguishable bosons and fermions.

018 qfull 02400 2 5 0 moderate thinking: exchange force and infsq well

Extra keywords: (Gr-185:5.5) and the infinite square well

5. Imagine two non-interacting particles in an infinite square in the range $[0, a]$. Recall the eigenfunctions for this case are

$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

for $n = 1, 2, 3, \dots$. Recall also the results of the Gr-182 and Gr-29:2.5 questions.

- Say the particles are distinguishable and are in states n and m . What is $\langle \Delta x^2 \rangle = \langle (x_1 - x_2)^2 \rangle$ for this case? What is it if $n = m$?

- b) Say the particles are identical bosons/fermions and are in the only allowed combination of states n and m . What is $\langle \Delta x^2 \rangle = \langle (x_1 - x_2)^2 \rangle$ for this case? What is it if $n = m$?

018 qfull 02500 2 3 0 mod math: coupled harmonic oscillator

Extra keywords: two identical particles, exact solution

6. There are two particles subject to separate simple harmonic oscillator (SHO) potentials. They are also coupled by a SHO interaction. The full Hamiltonian is:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}m_1\omega^2 x_1^2 + \frac{1}{2}m_2\omega^2 x_2^2 + \frac{1}{2}k(x_1 - x_2)^2 ,$$

where $k > 0$ which in this context means the interaction is attractive.

- Transform to the center-of-mass-relative (CM-REL) coordinates (showing all the steps) and show that the Hamiltonian separates into a center-of-mass (CM) SHO Hamiltonian and a relative (REL) SHO Hamiltonian. Does the problem have an exact solution? Write down the general expression for the eigen-energies of the total stationary states in terms of the SHO quantum numbers n_{CM} and n_{REL} for the respective CM and REL parts. Define $\tilde{\omega}$ as the angular frequency of the REL energies.
- Next write the expression for the eigen-energies in the case that $k = 0$. Define a new quantum number n that alone gives the eigen-energy and the degeneracy of the eigen-energy. What is the degeneracy of an eigen-energy of quantum number n .
- Now assume that $k > 0$, but that $k/(\mu\omega^2) \ll 1$. Write down a first order correct expression for the energy in terms of n and n_{REL} . Give a schematic energy-level diagram.
- Now assume that $k/(\mu\omega^2) \gg 1$. Give a schematic energy-level diagram in this case.
- Now assume that the two particles are identical spin-0 bosons. Note that identical means they now have the same mass. Given the symmetry requirement for boson states, which solutions (specified by the n_{CM} and n_{REL} quantum numbers) are not physically allowed?
- Now assume that the two particles are identical spin-1/2 fermions. Note again that identical means they now have the same mass. But also note they aren't electrons. Their interactions are determined by the given Hamiltonian only. Because the particles are spin-1/2 fermions, the eigen wave functions for system must be multiplied by appropriate eigen-spinors to specify the full eigenstate. Given the antisymmetry requirement for fermion states, what restrictions are put on the wave function and spinor quantum numbers of an eigenstate?

018 qfull 02600 1 5 0 easy thinking: symmetrization, Slater determinant

Extra keywords: (Gr-187:5.7)

7. Say that you solve a Schrödinger equation for N identical particles to get the normalized wave function $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N)$. How would you symmetrize the wave function for bosons? Then how would you symmetrize for fermions all in the spin-up state so that you don't have spinors to complicate the question? How would you normalize the wave function?

018 qfull 02700 1 5 0 easy thinking: doubly excite He decay

Extra keywords: (Gr188.58a)

8. Say you put two electrons into the $n = 2$ principle quantum number shell of a neutral helium atom and immediately one electron is ejected and the other decays to the ground of the He^+ ion. What approximately is the kinetic energy of the ejected electron. **NOTE:** Without a detailed specification of the doubly-excited helium atom we cannot know exactly what the energies of the excited electrons are. There are two simple approximate choices for their energies: 1) assume that the energy levels of the singly-excited helium atom apply (see, e.g., Gr-189); 2) assume that the $Z = 2$ hydrogenic energy levels apply. The first choice is probably most in error because it

assumes too much electron-electron interaction: the electrons may further apart in the actual doubly-excited state; but in fact where they are depends on exactly what doubly excited state they are in. The 2nd choice is certainly wrong by assuming zero electron-electron interaction.

018 qfull 02800 1 5 0 easy thinking: spectrum of He II

Extra keywords: (Gr-188:58b)

9. Describe the spectrum of He II (i.e., singly-ionized helium or He^+) sans perturbations..

018 qfull 02900 2 5 0 moderate thinking: helium with bosons

Extra keywords: (Gr-188:5.9)

10. Describe qualitatively how the helium atom energy level diagram would plausibly change under the following conditions.
- Say the electrons were spin zero bosons.
 - Say the electrons were spin 1/2 bosons—a contradiction in postulates, but for the sake of argument have it so.
 - Say the electrons were spin 1/2 fermions, but were quantum mechanically distinguishable particles. **HINT:** In this case the answer is going to be pretty much indefinite.

018 qfull 03000 3 3 0 tough math: helium atom 1st order perturbation

Extra keywords: (Gr-188:5.10)

11. If one neglects the electron-electron interaction of the helium atom then the spatial ground state is just the product of two hydrogenic states:

$$\psi(\vec{r}_1, \vec{r}_2) = \psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2) = \frac{1}{\pi a_{\text{He}}^3/8} e^{-2(r_1+r_2)/a} = \frac{8}{\pi a^3} e^{-2(r_1+r_2)/a} ,$$

where $a_{\text{He}} = a/Z = a/2$ is the helium Bohr radius and a is the standard Bohr radius (see, e.g., Gr-137–138 and Gr-187). The 1st order perturbation correction to the helium atom ground state is given by

$$\langle H' \rangle ,$$

where H' is the perturbation Hamiltonian: i.e.,

$$\frac{e^2}{4\pi\epsilon_0} \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

in MKS units (see, e.g., Gr-187) or

$$\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

in Gaussian CGS units. Note that we use e for both fundamental charge unit and the exponential factor: this is conventional of course: context must decide which is which.

- a) Analytically calculate

$$\left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle .$$

HINTS: Set

$$|\vec{r}_1 - \vec{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1r_2\mu} ,$$

where $\mu = \cos\theta$ is the angle cosine between the vectors. Integrate over all \vec{r}_2 space first taking \vec{r}_1 as the z axis for spherical coordinates. It helps to switch to dimensionless variables earlier on. There are no special difficulties or tricks: just a moderate number of steps that have to be done with tedious care.

b) Now the expression for a hydrogenic energy level, sans perturbations, is

$$E_n = -\frac{1}{2}m_e c^2 \alpha^2 \frac{Z^2}{n^2} = -\frac{Z^2 E_{\text{ryd}}}{n^2} \approx -\frac{13.6 Z^2}{n^2} \text{ eV} ,$$

where m_e is the electron mass, α is the fine structure constant, Z is the nuclear charge, and $E_{\text{ryd}} \approx 13.6 \text{ eV}$ is the Rydberg energy (see, e.g., Ga-197). In Gaussian CGS units

$$\alpha = \frac{e^2}{\hbar c} \quad \text{and} \quad a = \frac{\hbar}{m_e c \alpha}$$

(e.g., Ga-199). What is the energy of the helium atom ground state in terms of Rydberg energies and eVs?

Chapt. 19 Solids

Multiple-Choice Problems

Full-Answer Problems

019 qfull 00100 2 5 0 moderate thinking: free electron metal

Extra keywords: (Ha-324:2.4)

1. Let us consider a free electron metal in 1, 2, and 3 dimensions simultaneously. Use periodic boundary conditions and assume “cubical” shape in all three cases. Let L be the length of a side of the “cube.”
 - a) Solve the time-independent Schrödinger equation for the stationary states for all three cases. Normalize the solutions and give their quantization requirements.
 - b) What is $\rho(k)$: i.e., the density of states per unit volume per unit (radial) wave number in the continuum of states approximation. Note that (radial) wave number is defined

$$k = \sqrt{\sum_j^{\ell} k_j^2} ,$$

where ℓ the number of dimensions. **HINT:** Remember that spatial states are doubly degenerate because of the 2 internal spin states of spin-1/2 particles.

- c) What is $\rho(E)$: i.e., the density of states per unit volume per unit energy in the continuum of states approximation. **HINT:** One requires the same number of states between any corresponding limits: i.e.,

$$\rho(k) dk = \rho(E) dE .$$

019 qfull 00200 2 5 0 moderate thinking: computing Fermi energies

Extra keywords: (Ha-324:2.3) free electron metals

2. The metals Na, Mg, and Al have, respectively 1, 2, and 3 free electrons per atom and volumes per atom 39.3 \AA^3 , 23.0 \AA^3 , and 16.6 \AA^3 . At zero temperature what is the Fermi energy to which the free electron states are filled?

Chapt. 20 Ephemeral Problems

Multiple-Choice Problems

Full-Answer Problems

030 qfull 00100 2 5 0 moderate thinking: eph Bose-Einstein condensate

Extra keywords: Greiner et al. 2002, 415, 39 with Stoof review on p. 25

1. Go to the library 2nd floor reading room and find the 20002jan03 issue of *Nature* (it may have been placed under the display shelf) and read the commentary article by Stoof on page 25 about a quantum phase transition from a Bose-Einstein condensate to a Mott insulator. What do you think Stoof really means when he says in the superfluid state “atoms still move freely from one valley to the next”? **NOTE:** The instructor disavows any ability to completely elucidate this commentary or the research article by Greiner et al. it comments on.

030 qfull 00200 2 3 0 moderate thinking: eph quantum gravity well

Extra keywords: reference: Nesvizhevsky et al. 2002, *Nature*, 413, 297

2. Is the gravity subject to quantum mechanical laws or is it somehow totally decoupled? Everyone really assumes that gravity is subject to quantum mechanical laws, but the assumption is not well verified experimentally: in fact it may never have been verified at all until now—not that I would know. The lack of experimental verification is because gravity is so infernally weak compared to other forces in microscopic experiments that it is usually completely negligible. Recently Nesvizhevsky et al. (2002, *Nature*, 413, 297) have reported from an experiment that a gravity well (at least part of the constraining potential is gravitational) does have quantized energy states. This appears to be the first time that such an experimental result has been achieved. It’s a wonderful result. Of course, if they hadn’t found quantization, it would have been a shock and most people would have concluded that the experiment was wrong somehow. Experiment may be the ultimate judge of theory, but experiment can certainly tell fibs for awhile.

Go read Nesvizhevsky et al. in the 2nd floor reading room of the library: the relevant issue may be under the shelf. If a neutron in the theoretically predicted gravity well made a transition from the 1st excited state to the ground state and emitted a photon, what would be the wavelength of the photon? Could such a photon be measured? What classically does such a transition correspond to?

030 qfull 00300 1 5 0 easy thinking: eph quantum computing

Extra keywords: Reference Seife, C. 2001, *Science*, 293, 2026

3. Read the article on quantum computing by Seife (2001, *Science*, 293, 2026) and make an estimate of how long it will be before there is a quantum computer that solves a computational problem not solvable by a classical computer: I’m excepting, of course, any problems concerning quantum computer operation itself. Give your reasoning. All answers are right—and wrong—or in a superposition of those two states. My answer is 1 year. **HINT:** You can probably find the

issue in the library, but there's one in the physics lounge near the Britney issue. Primers on quantum computing can be found by going to

<http://www.physics.unlv.edu/~jeffery/images/science>

and clicking down through quantum mechanics and quantum computing.

030 qfull 00400 2 5 0 moderate thinking: eph C-70 diffraction

Extra keywords: Reference Nairz et al. 2001, quant-ph/0105061

4. On the web go to the Los Alamos eprint archive:

<http://xxx.lanl.gov/> .

There click on search and then on search for articles by Zeilinger under the quant-ph topic. Locate Nairz, Arndt, & Zeilinger 2001, quant-ph/0105061 and download it. This is article reports the particle diffraction for C₇₀ (a fullerene). There should be great pictures on the web of fullerenes, but the best I could find were at

<http://www.sussex.ac.uk/Users/kroto/fullgallery.html>

and

<http://cnst.rice.edu/pics.html>

and these don't have descriptions. Fullerenes are the largest particles ever shown to diffract: their size scale must be order-of a nanometer: 10 times ordinary atomic size. The article calls itself a verification of the Heisenberg uncertainty principle. In a general sense this is absolutely true since they verify the wave nature of particle propagation. But it isn't a direct test of the formal uncertainty relation

$$\sigma_x \sigma_{p_x} \geq \frac{\hbar}{2} ,$$

where σ_x and σ_{p_x} are standard deviations of x -direction position and momentum, respectively, for the wave function (e.g., Gr-18, Gr-108–110). Explain why it isn't a direct test. **HINTS:** You should all have studied physical optics at some point. Essentially what formula are they testing?

030 qfull 00500 1 5 0 easy thinking: bulk and branes

Extra keywords: Reference Arkani-Hamed, N., et al. 2002, Physics Today, February, 35

5. Go the library basement and read the article by Arkani-Hamed et al. (Physics Today, February, p. 35). Perhaps a 2nd reading would help or a course in particle physics. Anyway what is the bulk (not Hulk, bulk) and the brane (not Brain, brane)?

030 qfull 00600 1 5 0 easy thinking: sympathetic cooling

Extra keywords: O'Hara & Thomas, 2001, Science, March 30, 291, 2556

6. Go to the library or the physics lounge and read O'Hara & Thomas (2001, Science, March 30, 291, p. 2556) on degenerate gases of bosons and fermions. What is sympathetic cooling?

Appendix 1 Mathematical Problems

Multiple-Choice Problems

Full-Answer Problems

031 qfull 00100 2 3 0 moderate math: Gauss summations

1. Gauss at the age of two proved various useful summation formulae. Now we can do this too maybe.

a) Prove

$$S_0(n) = \sum_{\ell=1}^n 1 = n .$$

HINT: This is really very easy.

b) Prove

$$S_1(n) = \sum_{\ell=1}^n \ell = \frac{n(n+1)}{2} .$$

HINT: The trick is to add to every term in the sum its “complement” and then sum those 2-sums and divide by 2 to account for double counting.

c) Prove

$$S_2(n) = \sum_{\ell=1}^n \ell^2 = \frac{n(n+1)(2n+1)}{6} .$$

HINT: A proof by induction works, but for that proof you need to know the result first and that’s the weak way. The stronger way is to reduce the problem to an already solved problem. Consider the general summation formula

$$S_k(n) = \sum_{\ell=1}^n \ell^k .$$

For each ℓ , you can construct a column of ℓ^{k-1} ’s that is ℓ in height. Can you add up the values in the table that is made up of these columns in some way to get $S_k(n)$.

d) Prove

$$S_3(n) = \sum_{\ell=1}^n \ell^3 = \frac{n^2(n+1)^2}{4} .$$

HINT: This formula can be proven using the “complement” trick and the formulae of parts (b) and (c). It can also more tediously be solved by the procedure hinted at in part (c). Or, of course, induction will work.

031 qfull 00200 1 3 0 easy math: uniqueness of power series

2. Power series are unique.

a) Prove that coefficients a_k of the power series

$$P(x) = \sum_{k=0}^{\infty} a_k x^k$$

are unique choices given that the series is convergent of course. **HINT:** The m th derivative of $P(x)$ evaluated at $x = 0$ can have only one value.

b) Prove that coefficients $a_{k\ell}$ of the double power series

$$P(x, y) = \sum_{k=0, \ell=0}^{\infty, \infty} a_{k\ell} x^k y^\ell$$

are unique choices given that the series is convergent of course. **HINT:** *Mutatis mutandis*.

031 qfull 00300 2 5 0 moderate thinking: biderivative formula proof

3. Prove the biderivative formula

$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^n \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}}$$

by induction.

031 qfull 00400 2 5 0 moderate thinking: integrals of type $x e^{-\lambda x^2}$

4. In evaluating anything that depends on a Gaussian distribution (e.g., the Maxwell-Boltzmann distribution of classical statistical mechanics), one frequently has to evaluate integrals of the type

$$I_n = \int_0^{\infty} x^n e^{-\lambda x^2} dx,$$

where n is an odd positive integer.

a) Solve for I_1 .

b) Obtaining the general formula for I_n is now trivial with a magic trick. Act on I_1 with the operator

$$\left(-\frac{d}{d\lambda} \right)^{(n-1)/2}.$$

c) From the general formula evaluate I_1 , I_3 , I_5 , and I_7 .

031 qfull 01000 2 5 0 moderate thinking:

5. In understanding determinants some permutation results must be proven. The proofs are expected to be cogent and memorable rather than mathematical rigorous.

a) Given n objects, prove that there are $n!$ permutations for ordering them in a line.

b) If you interchange any two particles in a given permutation, you get another permutation. Let's call that action an exchange. If you exchange nearest nearest neighbors, let's call that a nearest neighbor or NN exchange. Prove that any exchange requires an odd number of NN exchanges.

c) Permutations have definite parity. This means that going from one definite permutation to another definite permutation by any possible series of NN exchanges (i.e., by any possible

path) will always involve either an even number of NN exchanges or an odd number: i.e., if one path is even/odd, then any other path is even/odd. Given that definite parity is true prove that any path of NN exchanges from a permutation that brings you back to that permutation (i.e., a closed path) has an even number of NN exchanges.

- d) Now we have to prove definite parity exists. Say there is a fiducial permutation which by definition we say has even parity. If definite parity exists, then every other permutation is definitely even or odd relative to the fiducial permutation. If $n = 1$, does definite parity hold in this trivial case? For $n \geq 2$, prove that definite parity holds. **HINTS:** It suffices to prove that going from the fiducial permutation to any other permutation always involves a definite even or odd path since the fiducial permutation is arbitrary. Proof by induction might be the best route. I can't see how brief word arguments can be avoided.
- e) Now prove for $n \geq 2$ that there are an equal number of even and odd permutations. **HINT:** Consider starting with an even permutation and systematically by an NN exchange path going through all possible permutations. Then start with an odd permutation and follow the same NN exchange path.

Appendix 2 Quantum Mechanics Equation Sheet

Note: This equation sheet is intended for students writing tests or reviewing material. Therefore it is neither intended to be complete nor completely explicit. There are fewer symbols than variables, and so some symbols must be used for different things.

1 Constants not to High Accuracy		
Constant Name	Symbol	Derived from CODATA 1998
Bohr radius	$a_{\text{Bohr}} = \frac{\lambda_{\text{Compton}}}{2\pi\alpha}$	$= 0.529 \text{ \AA}$
Boltzmann's constant	k	$= 0.8617 \times 10^{-6} \text{ eV K}^{-1}$ $= 1.381 \times 10^{-16} \text{ erg K}^{-1}$
Compton wavelength	$\lambda_{\text{Compton}} = \frac{h}{m_e c}$	$= 0.0246 \text{ \AA}$
Electron rest energy	$m_e c^2$	$= 5.11 \times 10^5 \text{ eV}$
Elementary charge squared	e^2	$= 14.40 \text{ eV \AA}$
Fine Structure constant	$\alpha = \frac{e^2}{\hbar c}$	$= 1/137.036$
Kinetic energy coefficient	$\frac{\hbar^2}{2m_e}$	$= 3.81 \text{ eV \AA}^2$
	$\frac{\hbar^2}{m_e}$	$= 7.62 \text{ eV \AA}^2$
Planck's constant	h	$= 4.15 \times 10^{-15} \text{ eV}$
Planck's h-bar	\hbar	$= 6.58 \times 10^{-16} \text{ eV}$
	hc	$= 12398.42 \text{ eV \AA}$
	$\hbar c$	$= 1973.27 \text{ eV \AA}$
Rydberg Energy	$E_{\text{Ryd}} = \frac{1}{2} m_e c^2 \alpha^2$	$= 13.606 \text{ eV}$

2 Schrödinger's Equation

$$H\Psi(x, t) = \left[\frac{p^2}{2m} + V(x) \right] \Psi(x, t) = i\hbar \frac{\partial \Psi(x, t)}{\partial t} \quad H\psi(x) = \left[\frac{p^2}{2m} + V(x) \right] \psi(x) = E\psi(x)$$

$$H\Psi(\vec{r}, t) = \left[\frac{p^2}{2m} + V(\vec{r}) \right] \Psi(\vec{r}, t) = i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} \quad H|\Psi\rangle = i\hbar \frac{\partial}{\partial t} |\Psi\rangle$$

$$H\psi(\vec{r}) = \left[\frac{p^2}{2m} + V(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r}) \quad H|\psi\rangle = E|\psi\rangle$$

3 Some Operators

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

$$H = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

$$p = \frac{\hbar}{i} \nabla \quad p^2 = -\hbar^2 \nabla^2$$

$$H = \frac{p^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})$$

$$\nabla = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} = \hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

4 Kronecker Delta and Levi-Civita Symbol

$$\delta_{ij} = \begin{cases} 1, & i = j; \\ 0, & \text{otherwise} \end{cases} \quad \varepsilon_{ijk} = \begin{cases} 1, & ijk \text{ cyclic}; \\ -1, & ijk \text{ anticyclic}; \\ 0, & \text{if two indices the same.} \end{cases}$$

$$\varepsilon_{ijk} \varepsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl} \quad (\text{Einstein summation on } i)$$

5 Time Evolution Formulae

$$\frac{d\langle A \rangle}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{\hbar} \langle i[H(t), A] \rangle \quad \text{General}$$

$$\frac{d\langle \vec{r} \rangle}{dt} = \frac{1}{m} \langle \vec{p} \rangle \quad \text{and} \quad \frac{d\langle \vec{p} \rangle}{dt} = -\langle \nabla V(\vec{r}) \rangle \quad \text{Ehrenfest's Theorem}$$

$$|\Psi(t)\rangle = \sum_j c_j(0) e^{-iE_j t / \hbar} |\phi_j\rangle$$

6 Simple Harmonic Oscillator (SHO) Formulae

$$V(x) = \frac{1}{2} m \omega^2 x^2 \quad \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \right) \psi = E \psi$$

$$\beta = \sqrt{\frac{m\omega}{\hbar}} \quad \psi_n(x) = \frac{\beta^{1/2}}{\pi^{1/4}} \frac{1}{\sqrt{2^n n!}} H_n(\beta x) e^{-\beta^2 x^2 / 2} \quad E_n = \left(n + \frac{1}{2} \right) \hbar \omega$$

$$H_0(\beta x) = H_0(\xi) = 1 \quad H_1(\beta x) = H_1(\xi) = 2\xi$$

$$H_2(\beta x) = H_2(\xi) = 4\xi^2 - 2 \quad H_3(\beta x) = H_3(\xi) = 8\xi^3 - 12\xi$$

7 Position, Momentum, and Wavenumber Representations

$$p = \hbar k \quad E_{\text{kinetic}} = E_T = \frac{\hbar^2 k^2}{2m} \quad |\Psi(p, t)|^2 dp = |\Psi(k, t)|^2 dk \quad \Psi(p, t) = \frac{\Psi(k, t)}{\sqrt{\hbar}}$$

$$x_{\text{op}} = x \quad p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad Q\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}, t\right) \quad \text{position representation}$$

$$x_{\text{op}} = -\frac{\hbar}{i} \frac{\partial}{\partial p} \quad p_{\text{op}} = p \quad Q\left(-\frac{\hbar}{i} \frac{\partial}{\partial p}, p, t\right) \quad \text{momentum representation}$$

$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{2\pi\hbar} dp \quad \delta(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{2\pi} dk$$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \Psi(p, t) \frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}} dp \quad \Psi(x, t) = \int_{-\infty}^{\infty} \Psi(k, t) \frac{e^{ikx}}{(2\pi)^{1/2}} dk$$

$$\Psi(p, t) = \int_{-\infty}^{\infty} \Psi(x, t) \frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{1/2}} dx \quad \Psi(k, t) = \int_{-\infty}^{\infty} \Psi(x, t) \frac{e^{-ikx}}{(2\pi)^{1/2}} dx$$

$$\Psi(\vec{r}, t) = \int_{\text{all space}} \Psi(\vec{p}, t) \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} d^3p \quad \Psi(\vec{r}, t) = \int_{\text{all space}} \Psi(\vec{k}, t) \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3k$$

$$\Psi(\vec{p}, t) = \int_{\text{all space}} \Psi(\vec{r}, t) \frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} d^3r \quad \Psi(\vec{k}, t) = \int_{\text{all space}} \Psi(\vec{r}, t) \frac{e^{-i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3r$$

8 Commutator Formulae

$$[A, BC] = [A, B]C + B[A, C] \quad \left[\sum_i a_i A_i, \sum_j b_j B_j \right] = \sum_{i,j} a_i b_j [A_i, B_j]$$

$$\text{if } [B, [A, B]] = 0 \quad \text{then } [A, F(B)] = [A, B]F'(B)$$

$$[x, p] = i\hbar \quad [x, f(p)] = i\hbar f'(p) \quad [p, g(x)] = -i\hbar g'(x)$$

$$[a, a^\dagger] = 1 \quad [N, a] = -a \quad [N, a^\dagger] = a^\dagger$$

9 Uncertainty Relations and Inequalities

$$\sigma_x \sigma_p = \Delta x \Delta p \geq \frac{\hbar}{2} \quad \sigma_Q \sigma_Q = \Delta Q \Delta R \geq \frac{1}{2} |\langle i[Q, R] \rangle|$$

$$\sigma_H \Delta t_{\text{scale time}} = \Delta E \Delta t_{\text{scale time}} \geq \frac{\hbar}{2}$$

10 Probability Amplitudes and Probabilities

$$\Psi(x, t) = \langle x | \Psi(t) \rangle \quad P(dx) = |\Psi(x, t)|^2 dx \quad c_i(t) = \langle \phi_i | \Psi(t) \rangle \quad P(i) = |c_i(t)|^2$$

11 Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \quad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos(\theta) \quad Y_{1,\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta) e^{\pm i\phi}$$

$$L^2 Y_{\ell m} = \ell(\ell+1) \hbar^2 Y_{\ell m} \quad L_z Y_{\ell m} = m \hbar Y_{\ell m} \quad |m| \leq \ell \quad m = -\ell, -\ell+1, \dots, \ell-1, \ell$$

0	1	2	3	4	5	6 ...
<i>s</i>	<i>p</i>	<i>d</i>	<i>f</i>	<i>g</i>	<i>h</i>	<i>i</i> ...

12 Hydrogenic Atom

$$\psi_{n\ell m} = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \quad \ell \leq n-1 \quad \ell = 0, 1, 2, \dots, n-1$$

$$a_z = \frac{a}{Z} \left(\frac{m_e}{m_{\text{reduced}}} \right) \quad a = \frac{\hbar}{m_e c \alpha} \quad \alpha = \frac{e^2}{\hbar c}$$

$$R_{10} = 2a_z^{-3/2} e^{-r/a_z} \quad R_{20} = \frac{1}{\sqrt{2}} a_z^{-3/2} \left(1 - \frac{1}{2} \frac{r}{a_z} \right) e^{-r/(2a_z)} \quad R_{21} = \frac{1}{\sqrt{24}} a_z^{-3/2} \frac{r}{a_z} e^{-r/(2a_z)}$$

$$R_{n\ell} = - \left\{ \left(\frac{2}{na_z} \right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^\ell L_{n+\ell}^{2\ell+1}(\rho) \quad \rho = \frac{2r}{nr_Z}$$

$$L_q(x) = e^x \left(\frac{d}{dx} \right)^q (e^{-x} x^q) \quad \text{Rodrigues' formula for the Laguerre polynomials}$$

$$L_q^j(x) = \left(\frac{d}{dx} \right)^j L_q(x) \quad \text{Associated Laguerre polynomials}$$

$$\langle r \rangle_{n\ell m} = \frac{a_Z}{2} [3n^2 - \ell(\ell+1)]$$

$$\text{Nodes} = (n-1) - \ell \quad \text{not counting zero or infinity}$$

$$E_n = -\frac{1}{2} m_e c^2 \alpha^2 \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} = -E_{\text{Ryd}} \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} = -13.606 \frac{Z^2}{n^2} \frac{m_{\text{reduced}}}{m_e} \text{ eV}$$

13 General Angular Momentum Formulae

$$[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k \quad (\text{Einstein summation on } k) \quad [J^2, \vec{J}] = 0$$

$$J^2 |jm\rangle = j(j+1) \hbar^2 |jm\rangle \quad J_z |jm\rangle = m \hbar |jm\rangle$$

$$J_{\pm} = J_x \pm iJ_y \quad J_{\pm}|jm\rangle = \hbar\sqrt{j(j+1) - m(m \pm 1)}|jm \pm 1\rangle$$

$$J_{\left\{ \begin{smallmatrix} x \\ y \end{smallmatrix} \right\}} = \left\{ \begin{smallmatrix} \frac{1}{2} \\ \frac{1}{2i} \end{smallmatrix} \right\} (J_+ \pm J_-) \quad J_{\pm}^{\dagger} J_{\pm} = J_{\mp} J_{\pm} = J^2 - J_z(J_z \pm \hbar)$$

14 Spin 1/2 Formulae

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle) \quad |\pm\rangle_y = \frac{1}{\sqrt{2}}(|+\rangle \pm i|-\rangle) \quad |\pm\rangle_z = |\pm\rangle$$

$$|++\rangle = |1, +\rangle|2, +\rangle \quad |+-\rangle = \frac{1}{\sqrt{2}}(|1, +\rangle|2, -\rangle \pm |1, -\rangle|2, +\rangle) \quad |--\rangle = |1, -\rangle|2, -\rangle$$

15 Time-Independent Approximation Methods

$$H = H^{(0)} + \lambda H^{(1)} \quad |\psi\rangle = N(\lambda) \sum_{k=0}^{\infty} \lambda^k |\psi_n^{(k)}\rangle$$

$$H^{(1)}|\psi_n^{(m-1)}\rangle(1 - \delta_{m,0}) + H^{(0)}|\psi_n^{(m)}\rangle = \sum_{\ell=0}^m E^{(m-\ell)}|\psi_n^{(\ell)}\rangle \quad |\psi_n^{(\ell>0)}\rangle = \sum_{m=0, m \neq n}^{\infty} a_{nm}|\psi_n^{(0)}\rangle$$

$$|\psi_n^{1\text{st}}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, k \neq n} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle$$

$$E_n^{1\text{st}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle$$

$$E_n^{2\text{nd}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle + \lambda^2 \sum_{\text{all } k, k \neq n} \frac{|\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$E(\phi) = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} \quad \delta E(\phi) = 0$$

$$H_{kj} = \langle \phi_k | H | \phi_j \rangle \quad H\vec{c} = E\vec{c}$$

16 Time-Dependent Perturbation Theory

$$\pi = \int_{-\infty}^{\infty} \frac{\sin^2(x)}{x^2} dx$$

17 Identical Particles

$$|a, b\rangle = \frac{1}{\sqrt{2}} (|1, a; 2, b\rangle \pm |1, b; 2, a\rangle)$$

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2))$$

Appendix 3 Multiple-Choice Problem Answer Tables

Note: For those who find scantrons frequently inaccurate and prefer to have their own table and marking template, the following are provided. I got the template trick from Neil Huffacker at University of Oklahoma. One just punches out the right answer places on an answer table and overlays it on student answer tables and quickly identifies and marks the wrong answers

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	6.	O	O	O	O	O
2.	O	O	O	O	O	7.	O	O	O	O	O
3.	O	O	O	O	O	8.	O	O	O	O	O
4.	O	O	O	O	O	9.	O	O	O	O	O
5.	O	O	O	O	O	10.	O	O	O	O	O

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	11.	O	O	O	O	O
2.	O	O	O	O	O	12.	O	O	O	O	O
3.	O	O	O	O	O	13.	O	O	O	O	O
4.	O	O	O	O	O	14.	O	O	O	O	O
5.	O	O	O	O	O	15.	O	O	O	O	O
6.	O	O	O	O	O	16.	O	O	O	O	O
7.	O	O	O	O	O	17.	O	O	O	O	O
8.	O	O	O	O	O	18.	O	O	O	O	O
9.	O	O	O	O	O	19.	O	O	O	O	O
10.	O	O	O	O	O	20.	O	O	O	O	O